RWTH AACHEN UNIVERSITY

Machine Learning – Lecture 19

Repetition

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Announcements

- Exams
  - Special oral exams (for exchange students):
    - We're in the process of sending out the exam slots
    - You'll receive an email with details tonight
    - Format: 30 minutes, 4 questions, 3 answers
  - Regular exams:
    - We will send out an email with the assignment to lecture halls
    - Format: 120min, closed-book exam

Announcements (2)

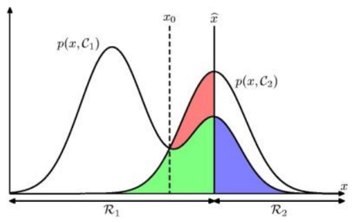
- Today, I'll summarize the most important points from the lecture.
  - It is an opportunity for you to ask questions…
  - …or get additional explanations about certain topics.
  - *So, please do ask.*
- Today's slides are intended as an index for the lecture.
  - But they are not complete, won't be sufficient as only tool.
  - Also look at the exercises – they often explain algorithms in detail.

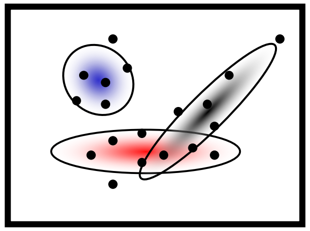
Announcements (3)

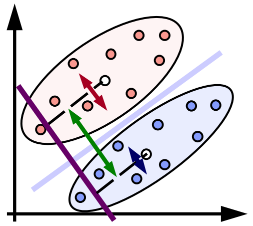
- Seminar in the summer semester
  - Current topics in Computer Vision and Machine Learning
  - Quick poll: Who is interested?

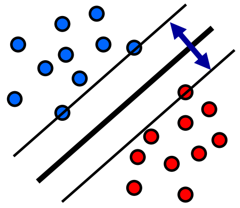
Course Outline

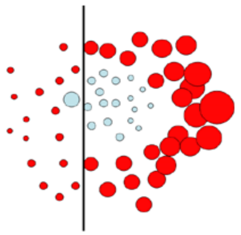
- Fundamentals
  - Bayes Decision Theory
  - Probability Density Estimation
  - Mixture Models and EM
- Classification Approaches
  - Linear Discriminants
  - Support Vector Machines
  - Ensemble Methods & Boosting
- Deep Learning
  - Foundations
  - Convolutional Neural Networks
  - Recurrent Neural Networks

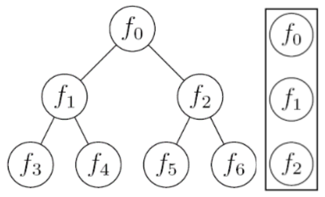


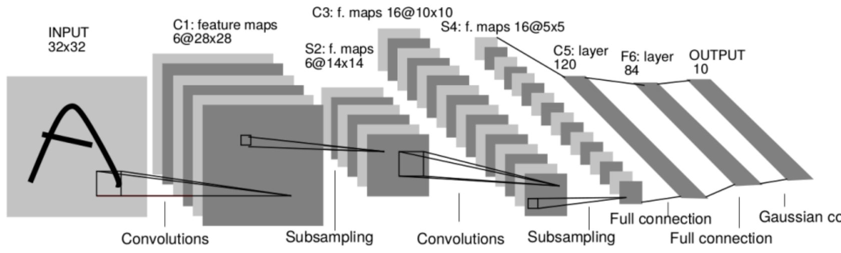




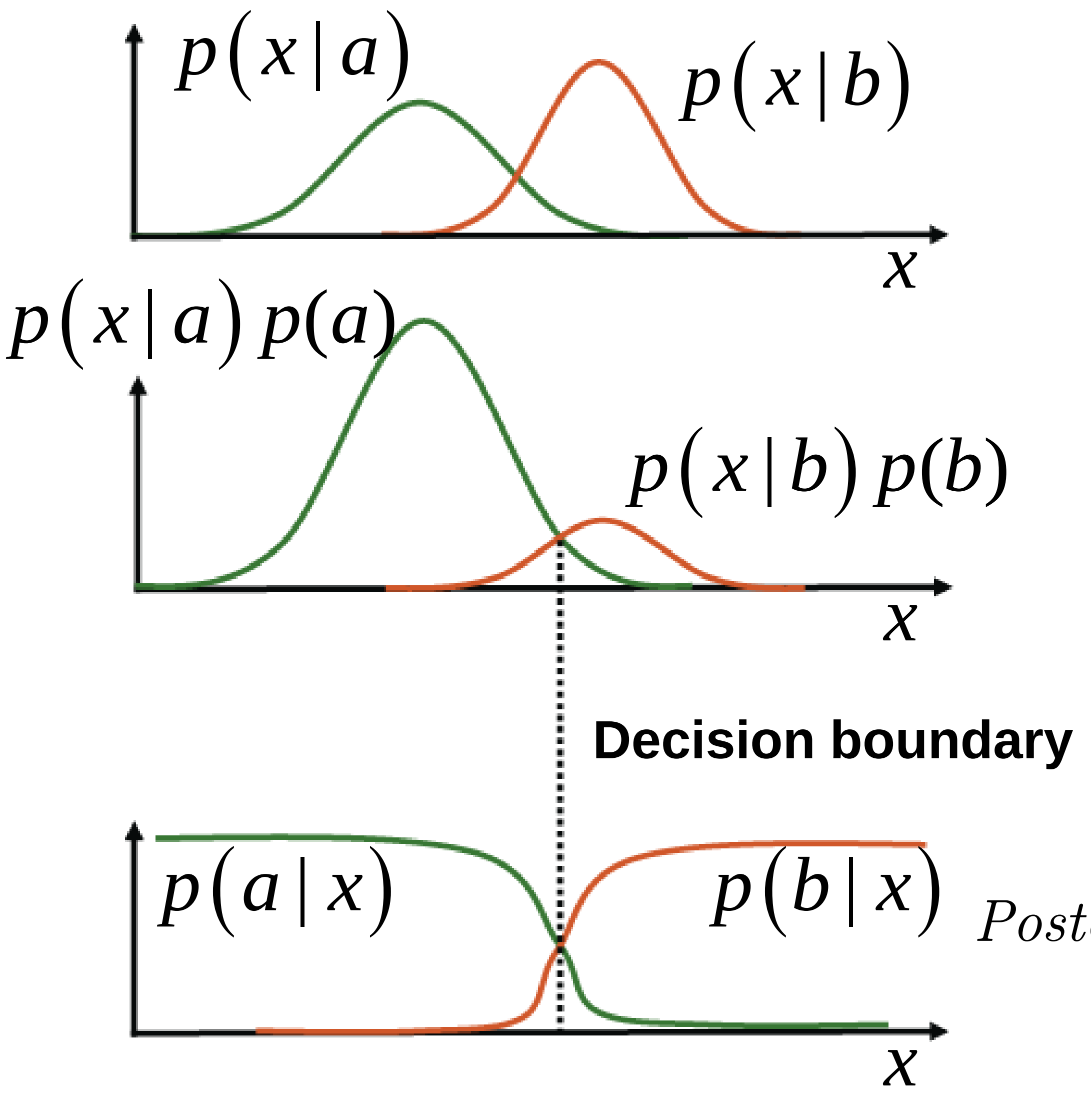








Recap: Bayes Decision Theory



$Likelihood$

$Likelihood \times Prior$

$$Posterior = \frac{Likelihood \times Prior}{NormalizationFactor}$$

Image source: C.M. Bishop, 2006

Recap: Bayes Decision Theory

- Optimal decision rule
  - Decide for C_1 if

$$p(\mathcal{C}_1|x) > p(\mathcal{C}_2|x)$$

  - This is equivalent to

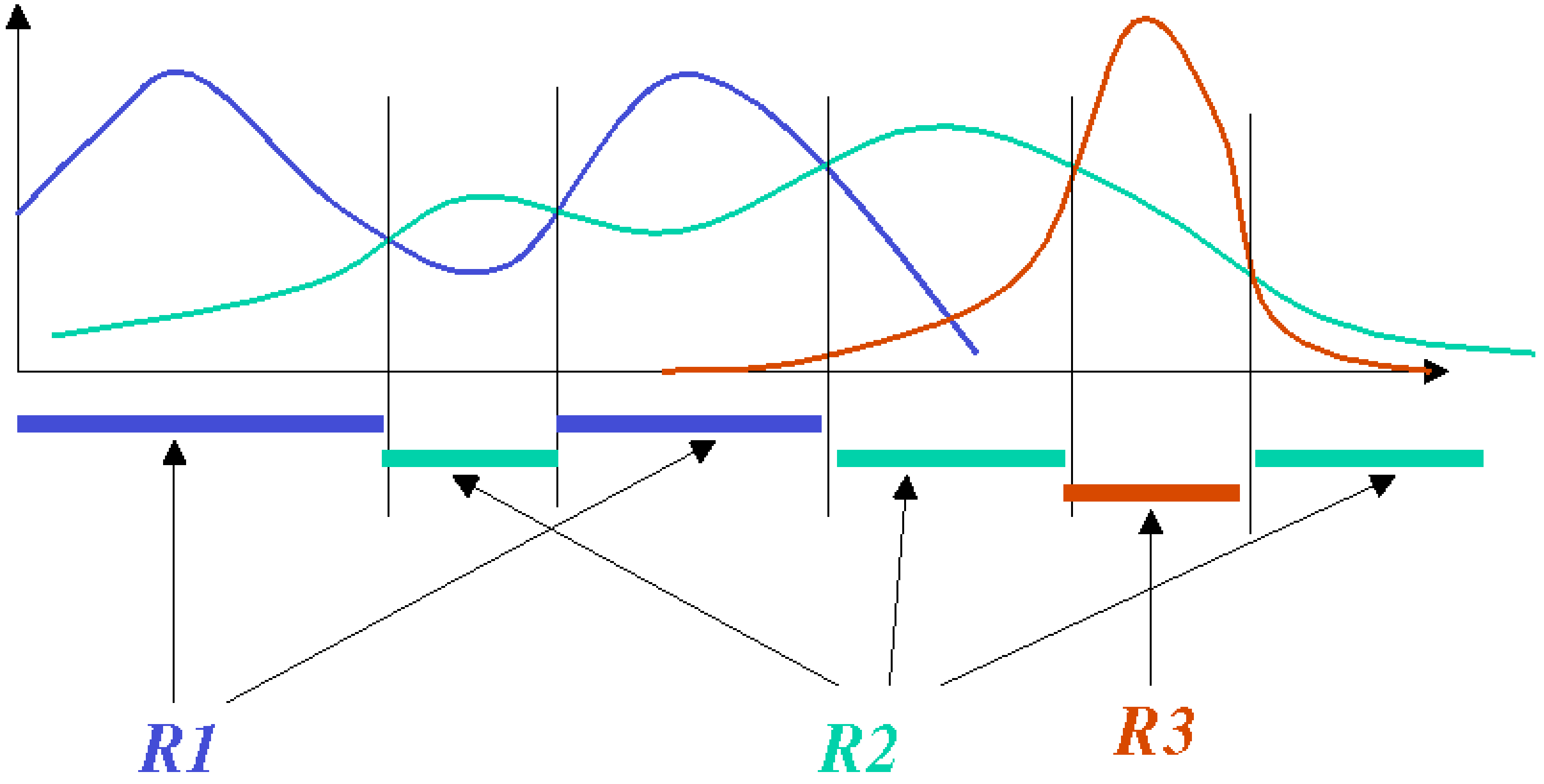
$$p(x|\mathcal{C}_1)p(\mathcal{C}_1) > p(x|\mathcal{C}_2)p(\mathcal{C}_2)$$

  - Which is again equivalent to (Likelihood-Ratio test)

$$\frac{p(x|\mathcal{C}_1)}{p(x|\mathcal{C}_2)} > \underbrace{\frac{p(\mathcal{C}_2)}{p(\mathcal{C}_1)}}_{\text{Decision threshold } \theta}$$

Recap: Bayes Decision Theory

- Decision regions: $\mathcal{R}_1$, $\mathcal{R}_2$, $\mathcal{R}_3$, …



Recap: Classifying with Loss Functions

- In general, we can formalize this by introducing a loss matrix L_{kj}

$$L_{kj} = \mathit{loss\ for\ decision}\ \mathcal{C}_j\ \mathit{if\ truth\ is}\ \mathcal{C}_k.$$

- Example: cancer diagnosis

$$L_{cancer\ \ diagnosis} = \text{Truth}\ \begin{array}{c|cc} & \multicolumn{2}{c}{\text{Decision}} \\ & \text{cancer} & \text{normal} \\ \hline \text{cancer} & 0 & 1000 \\ \text{normal} & 1 & 0 \end{array}$$

Recap: Minimizing the Expected Loss

see Exercise 1.3

- Optimal solution minimizes the loss.
  - But: loss function depends on the true class, which is unknown.
- Solution: Minimize the expected loss

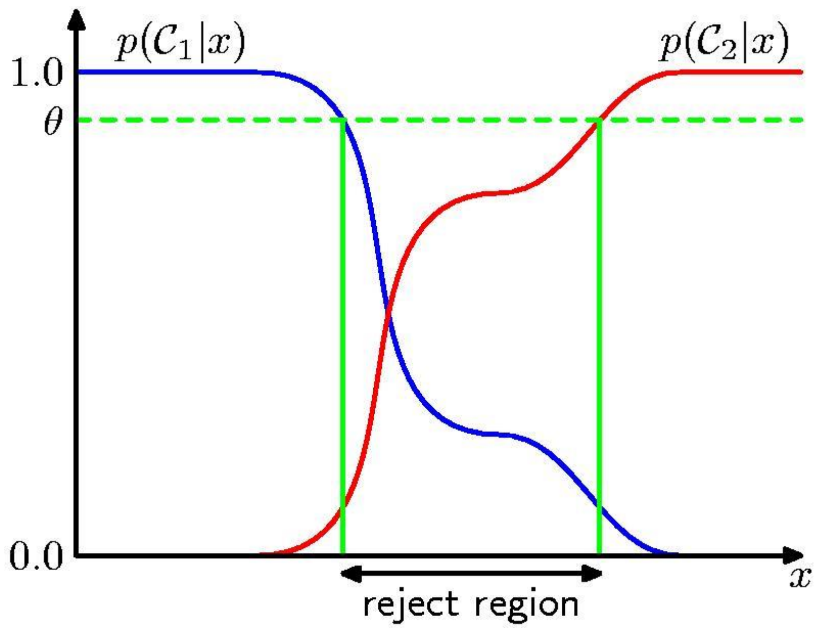
$$\mathbb{E}[L] = \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(\mathbf{x}, \mathcal{C}_k) \,\mathrm{d}\mathbf{x}$$

- This can be done by choosing the regions $\mathcal{R}_j$ such that

$$\mathbb{E}[L] = \sum_k L_{kj} p(\mathcal{C}_k|\mathbf{x})$$

which is easy to do once we know the posterior class probabilities $p(\mathcal{C}_k|\mathbf{x})$

Recap: The Reject Option



- Classification errors arise from regions where the largest posterior probability $p(\mathcal{C}_k|\mathbf{x})$ is significantly less than 1.
  - These are the regions where we are relatively uncertain about class membership.
  - For some applications, it may be better to reject the automatic decision entirely in such a case and e.g. consult a human expert.

Image source: C.M. Bishop, 2006

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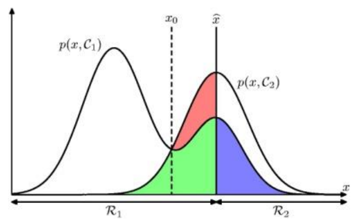
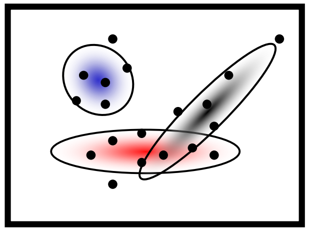
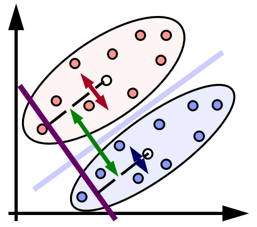
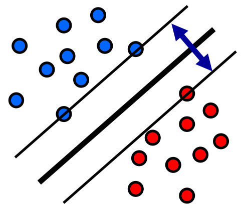
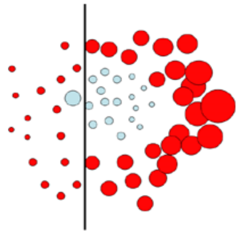
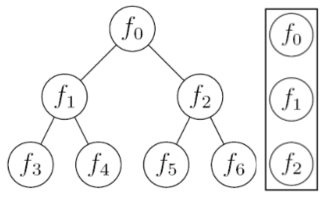


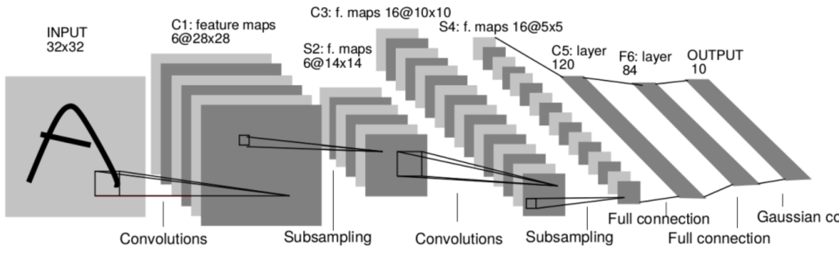








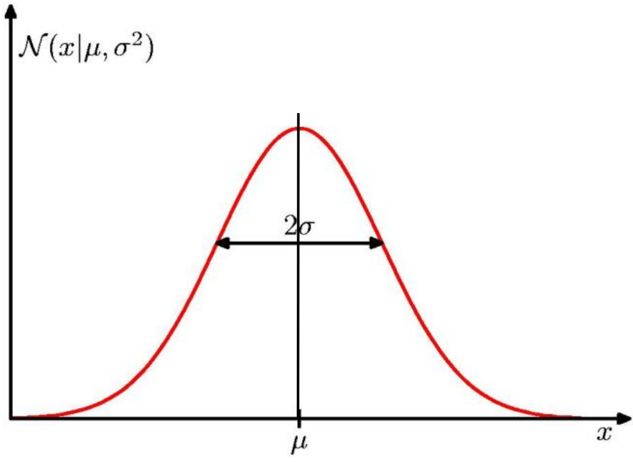




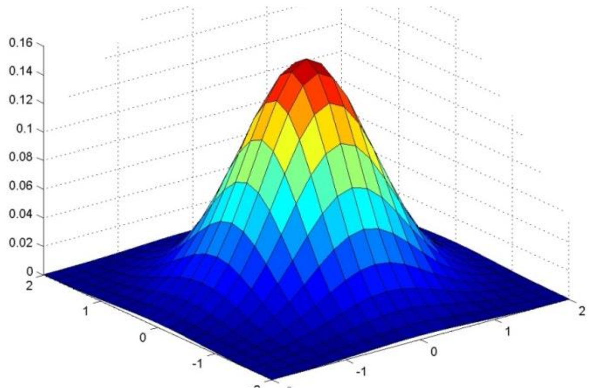
Recap: Gaussian (or Normal) Distribution

- One-dimensional case
  - Mean μ
  - Variance σ^2

$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$



- Multi-dimensional case
  - Mean μ
  - Covariance Σ



$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\mathbf{\Sigma}) = \frac{1}{(2\pi)^{D/2}|\mathbf{\Sigma}|^{1/2}}\exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

Image source: C.M. Bishop, 2006

Recap: Maximum Likelihood Approach

see Exercise 1.4

- Computation of the likelihood
  - Single data point: $p(x_n|\theta)$
  - Assumption: all data points $X = \{x_1, \ldots, x_n\}$e independent

$$L(\theta) = p(X|\theta) = \prod_{n=1}^{N} p(x_n|\theta)$$

  - Log-likelihood

$$E(\theta) = -\ln L(\theta) = -\sum_{n=1}^{N} \ln p(x_n|\theta)$$

- Estimation of the parameters θ (Learning)
  - Maximize the likelihood (= minimize the negative log-likelihood)

  $\Rightarrow$ Take the derivative and set it to zero.

$$\frac{\partial}{\partial\theta}E(\theta) = -\sum_{n=1}^{N} \frac{\frac{\partial}{\partial\theta}p(x_n|\theta)}{p(x_n|\theta)} \overset{!}{=} 0$$

Recap: Bayesian Learning Approach

- Bayesian view:
  - Consider the parameter vector θ as a random variable.
  - When estimating the parameters, what we compute is

$$p(x|X) = \int p(x, \theta|X) d\theta$$

Assumption: given θ, this doesn't depend on X anymore

$$p(x, \theta|X) = p(x|\theta, \cancel{X}) p(\theta|X)$$

$$p(x|X) = \int \underbrace{p(x|\theta)}_{} p(\theta|X) d\theta$$

This is entirely determined by the parameter θ (i.e. by the parametric form of the pdf).

Recap: Bayesian Learning Approach

- Discussion

Likelihood of the parametric form θ given the data set X.

Estimate for x based on parametric form θ

Prior for the parameters θ

$$p(x|X) = \int \frac{p(x|\theta)L(\theta)p(\theta)}{\underbrace{\int L(\theta)p(\theta)d\theta}} d\theta$$

Normalization: integrate over all possible values of θ

- The more uncertain we are about θ, the more we average over all possible parameter values.

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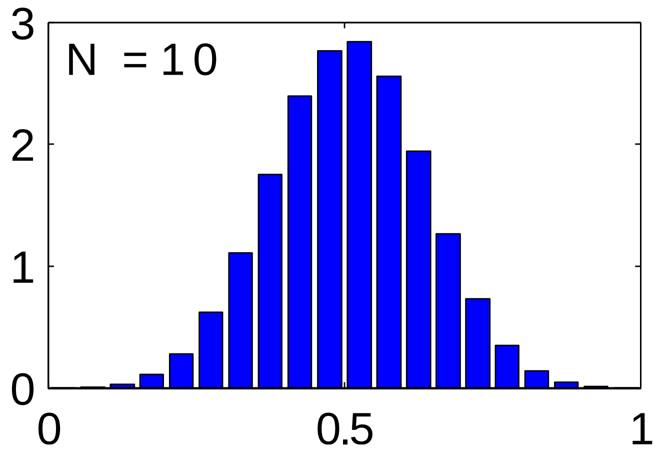
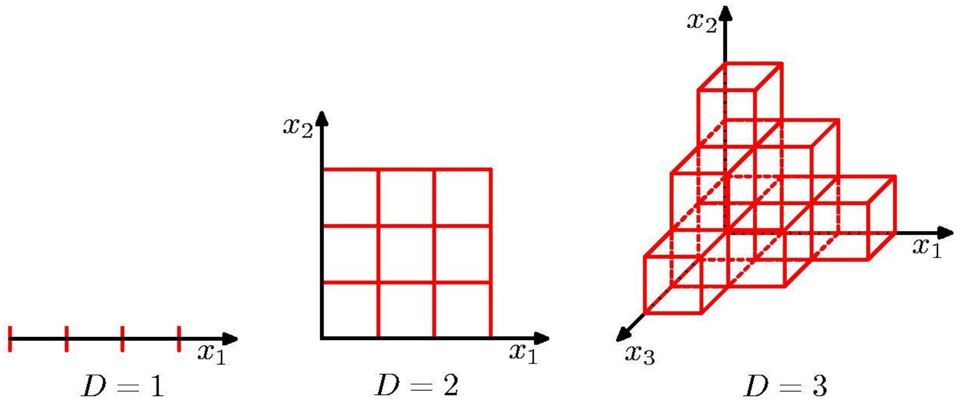
Recap: Histograms

- Basic idea:
  - Partition the data space into distinct bins with widths Δ_i and count the number of observations, n_i, in each bin.

$$p_i = \frac{n_i}{N\Delta_i}$$



  - Often, the same width is used for all bins, $\Delta_i = \Delta$.
  - This can be done, in principle, for any dimensionality D…



…but the required number of bins grows exponentially with D!

Image source: C.M. Bishop, 2006

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Recap: Kernel Density Estimation

see Exercise 1.5

- Approximation formula:

$$p(\mathbf{x}) \approx \frac{K}{NV}$$

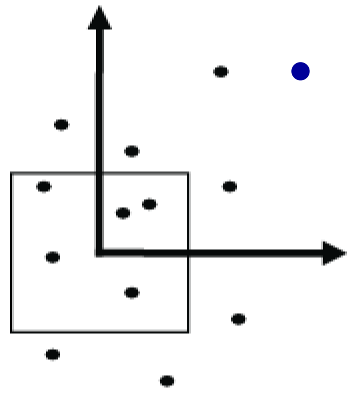
fixed V
determine K

fixed K
determine V

Kernel Methods

K-Nearest Neighbor

- Kernel methods
  - Place a *kernel window* k at location $\mathbf{x}$ and count how many data points fall inside it.



- K-Nearest Neighbor
  - Increase the volume V until the K next data points are found.

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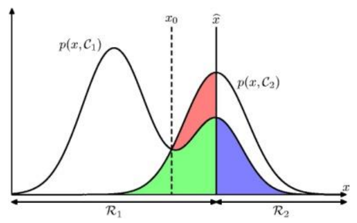
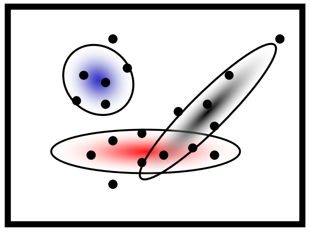
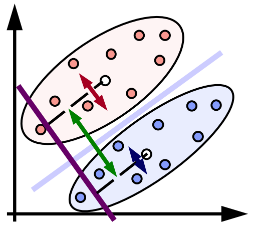
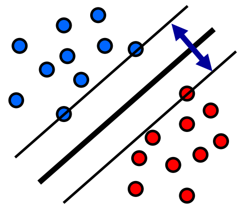
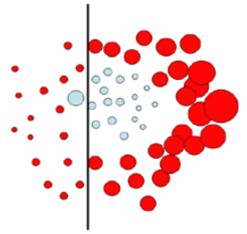
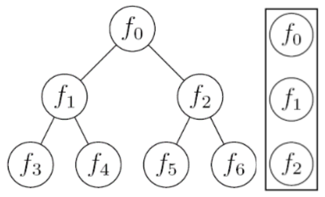


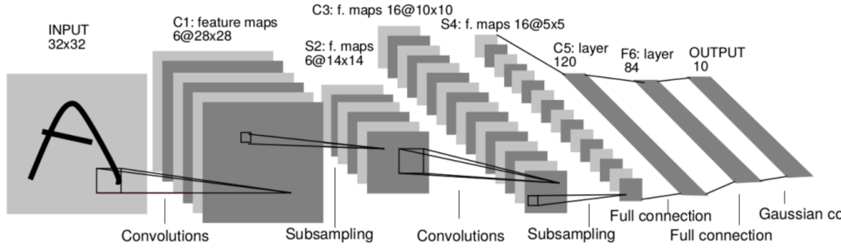






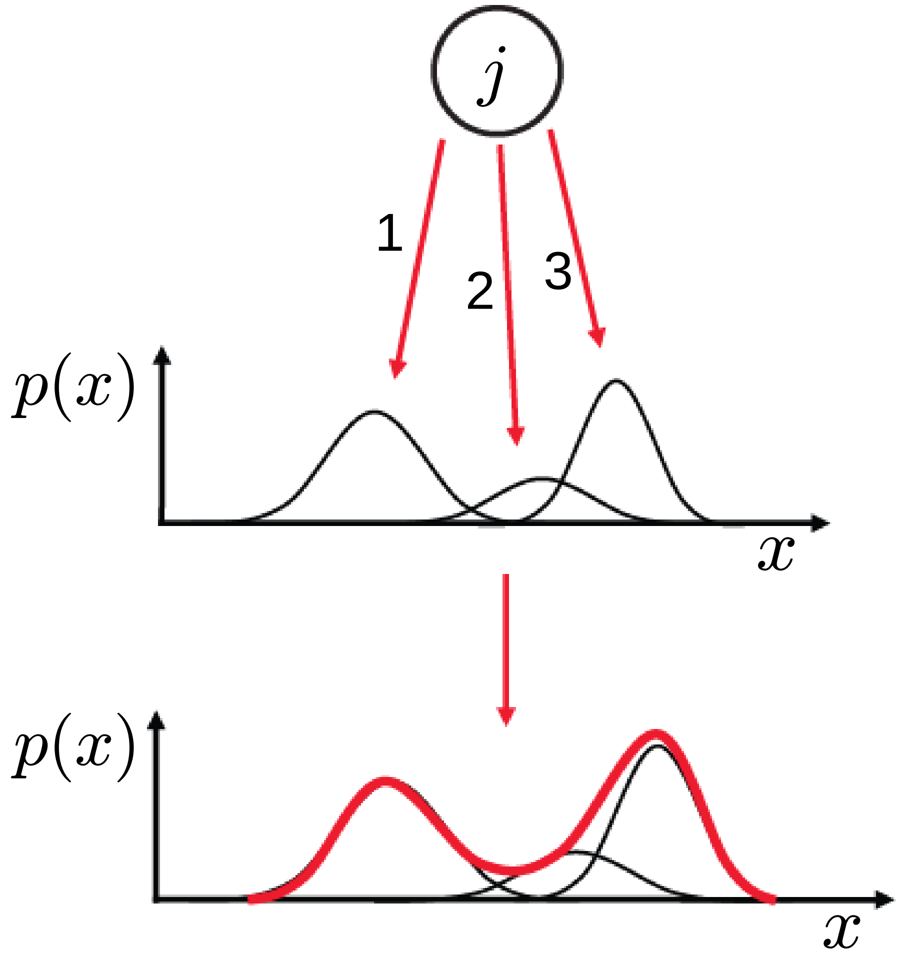






Recap: Mixture of Gaussians (MoG)

- "Generative model"



$p(j) = \pi_j$ "Weight" of mixture component

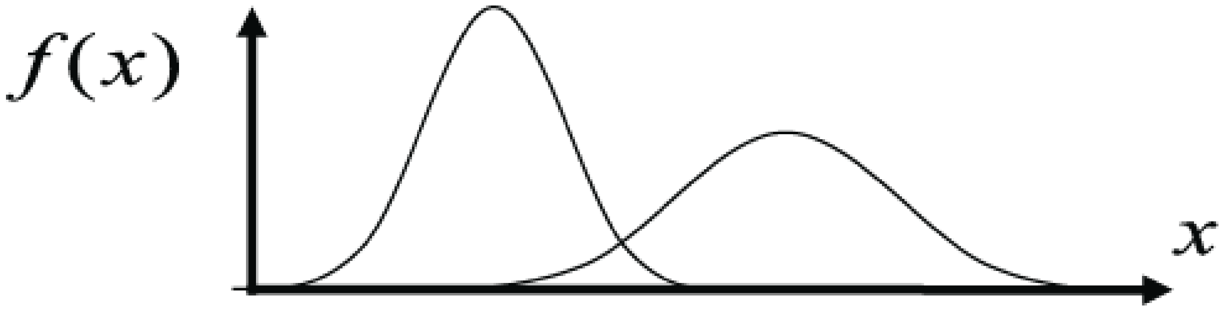
$p(x|\theta_j)$ Mixture component

Mixture density

$$p(x|\theta) = \sum_{j=1}^{M} p(x|\theta_j)p(j)$$

Recap: MoG – Iterative Strategy

- Assuming we knew the values of the hidden variable…



ML for Gaussian #1 ML for Gaussian #2

assumed known $\longrightarrow$ 1 111 22 2 2 j

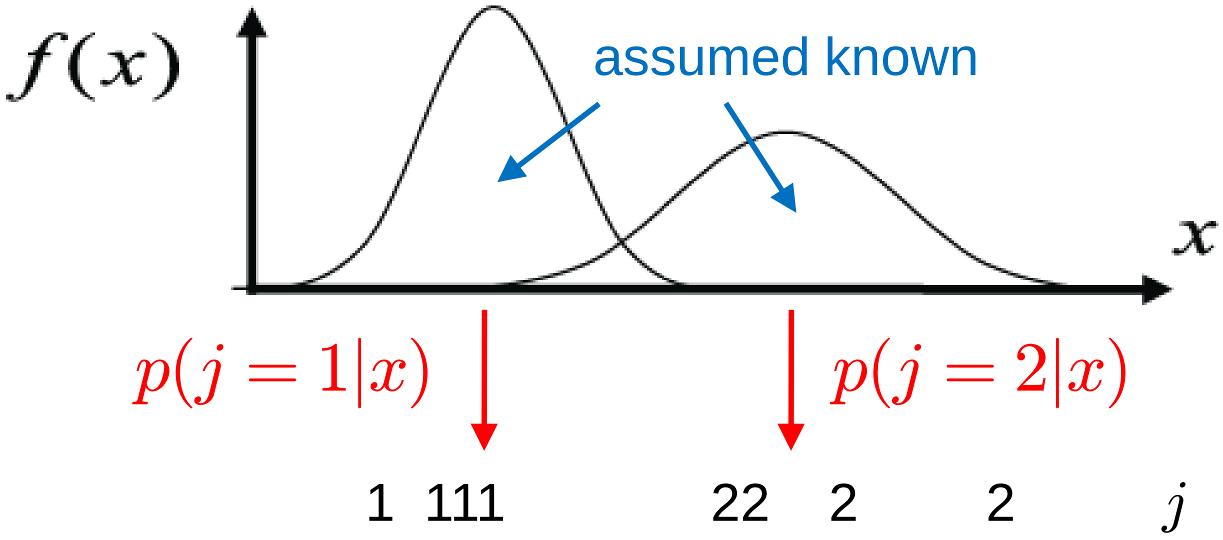
$$h(j=1|x_n) = \quad 1 \;\; 111 \qquad 00 \quad 0 \quad 0$$

$$h(j=2|x_n) = \quad 0 \;\; 000 \qquad 11 \quad 1 \quad 1$$

$$\mu_1 = \frac{\sum_{n=1}^{N} h(j=1|x_n)x_n}{\sum_{i=1}^{N} h(j=1|x_n)} \qquad \mu_2 = \frac{\sum_{n=1}^{N} h(j=2|x_n)x_n}{\sum_{i=1}^{N} h(j=2|x_n)}$$

Recap: MoG – Iterative Strategy

- Assuming we knew the mixture components…



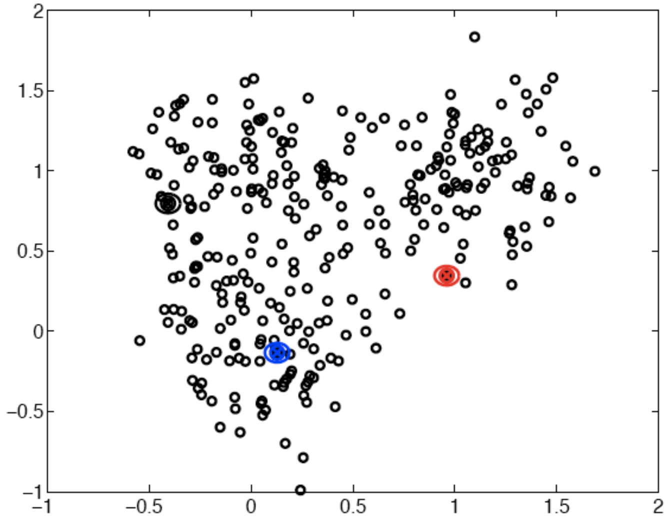
- Bayes decision rule: Decide $j = 1$ if

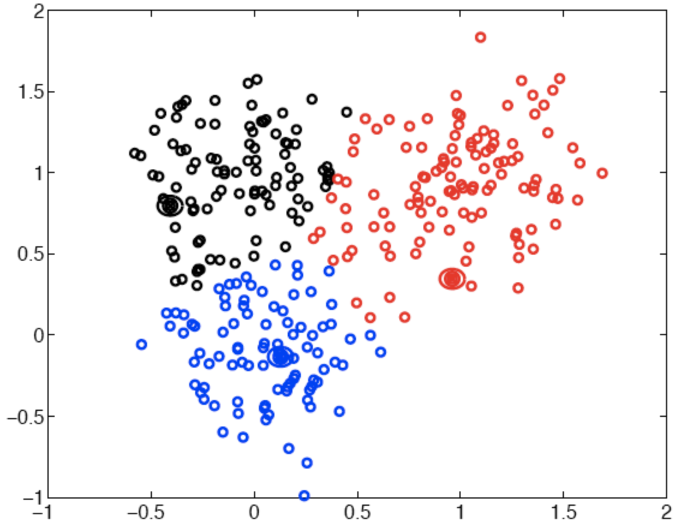
$$p(j = 1|x_n) > p(j = 2|x_n)$$

Recap: K-Means Clustering

- Iterative procedure
  1. Initialization: pick K arbitrary centroids (cluster means)
  2. Assign each sample to the closest centroid.
  3. Adjust the centroids to be the means of the samples assigned to them.
  4. Go to step 2 (until no change)

- Algorithm is guaranteed to converge after finite #iterations.
  - Local optimum
  - Final result depends on initialization.





Recap: EM Algorithm

see Exercise 1.6

- Expectation-Maximization (EM) Algorithm
  - E-Step: softly assign samples to mixture components

$$\gamma_j(\mathbf{x}_n) \leftarrow \frac{\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}{\sum_{k=1}^{N} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)} \qquad \forall j = 1, \ldots, K, \quad n = 1, \ldots, N$$

  - M-Step: re-estimate the parameters (separately for each mixture component) based on the soft assignments

$$\hat{N}_j \leftarrow \sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)$$ = soft number of samples labeled j

$$\hat{\pi}_j^{\text{new}} \leftarrow \frac{\hat{N}_j}{N}$$

$$\hat{\boldsymbol{\mu}}_j^{\text{new}} \leftarrow \frac{1}{\hat{N}_j} \sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)\mathbf{x}_n$$

$$\hat{\boldsymbol{\Sigma}}_j^{\text{new}} \leftarrow \frac{1}{\hat{N}_j} \sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)(\mathbf{x}_n - \hat{\boldsymbol{\mu}}_j^{\text{new}})(\mathbf{x}_n - \hat{\boldsymbol{\mu}}_j^{\text{new}})^{\mathrm{T}}$$

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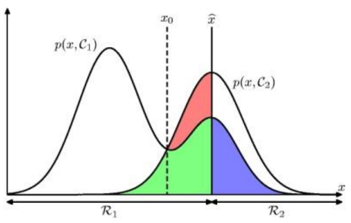
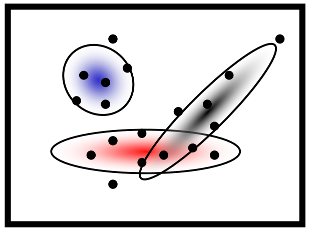
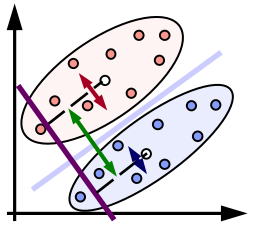
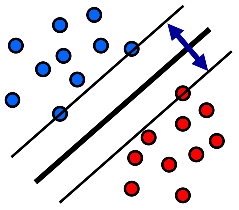
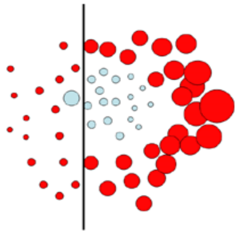
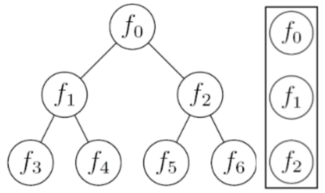


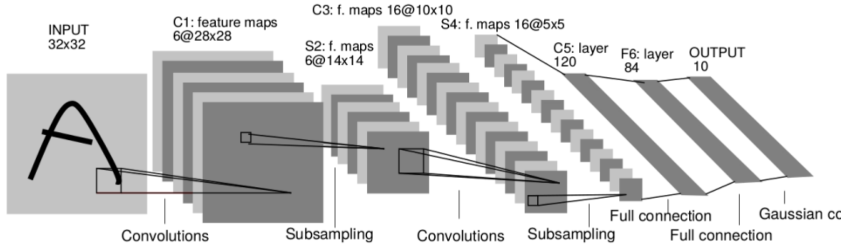












Recap: Linear Discriminant Functions

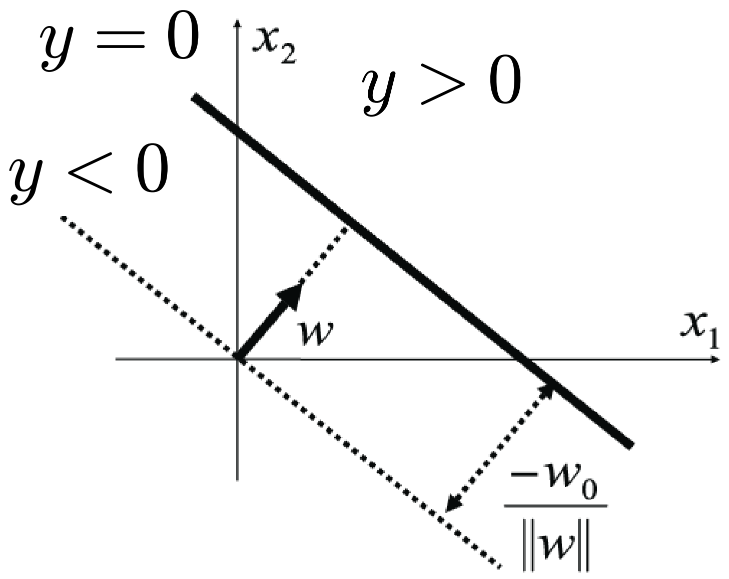
- Basic idea
  - Directly encode decision boundary
  - Minimize misclassification probability directly.

- Linear discriminant functions

$$y(\mathbf{x}) = \underbrace{\mathbf{w}}_{\text{weight vector}}^{\mathrm{T}}\mathbf{x} + \underbrace{w_0}_{\text{"bias" (= threshold)}}$$

weight vector

"bias"
(= threshold)



  - $\mathbf{w}$, w_0 define a hyperplane in $\mathbb{R}^D$.
  - If a data set can be perfectly classified by a linear discriminant, then we call it linearly separable.

Recap: Least-Squares Classification

see Exercise 2.1

- Simplest approach
  - Directly try to minimize the sum-of-squares error

$$E(\mathbf{w}) = \sum_{n=1}^{N} (y(\mathbf{x}_n; \mathbf{w}) - \mathbf{t}_n)^2$$

$$E_D(\widetilde{\mathbf{W}}) = \frac{1}{2}\mathrm{Tr}\left\{(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})^{\mathrm{T}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})\right\}$$

  - Setting the derivative to zero yields

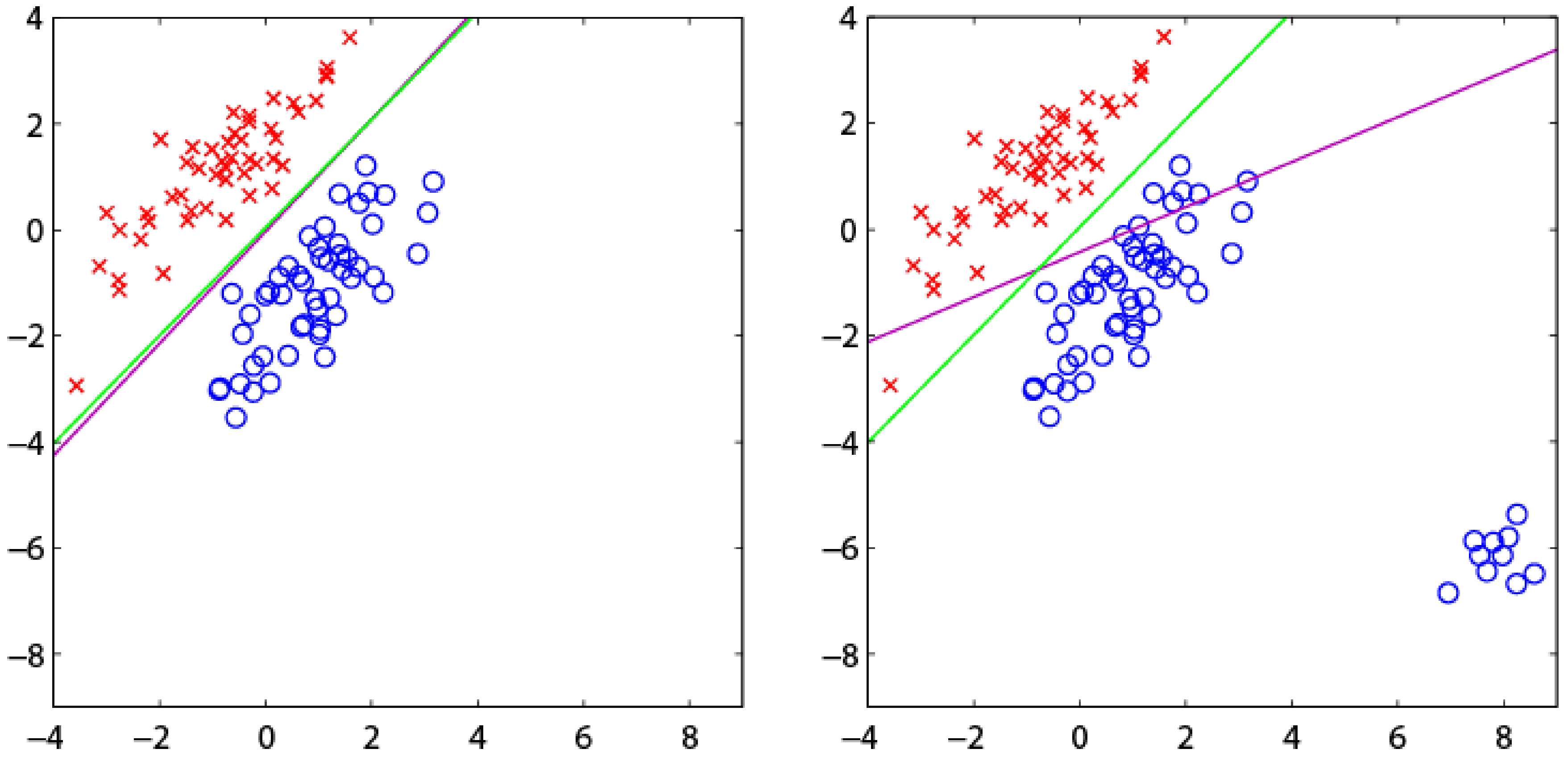
$$\widetilde{\mathbf{W}} = (\widetilde{\mathbf{X}}^{\mathrm{T}}\widetilde{\mathbf{X}})^{-1}\widetilde{\mathbf{X}}^{\mathrm{T}}\mathbf{T} = \widetilde{\mathbf{X}}^{\dagger}\mathbf{T}$$

  - We then obtain the discriminant function as

$$\mathbf{y}(\mathbf{x}) = \widetilde{\mathbf{W}}^{\mathrm{T}}\widetilde{\mathbf{x}} = \mathbf{T}^{\mathrm{T}}\left(\widetilde{\mathbf{X}}^{\dagger}\right)^{\mathrm{T}}\widetilde{\mathbf{x}}$$

  - $\Rightarrow$ Exact, closed-form solution for the discriminant function parameters.

Recap: Problems with Least Squares



- Least-squares is very sensitive to outliers!
  - The error function penalizes predictions that are "too correct".

Image source: C.M. Bishop, 2006

Recap: Generalized Linear Models

- Generalized linear model

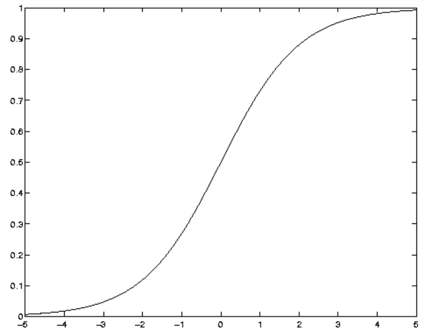
$$y(\mathbf{x}) = g(\mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0)$$

  - $g(\,\cdot\,)$ is called an activation function and may be nonlinear.
  - The decision surfaces correspond to

$$y(\mathbf{x}) = const. \quad \Leftrightarrow \quad \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0 = const.$$

  - If g is monotonous (which is typically the case), the resulting decision boundaries are still linear functions of $\mathbf{x}$.

- Advantages of the non-linearity
  - Can be used to bound the influence of outliers and "too correct" data points.
  - When using a sigmoid for $g(\cdot)$, we can interpret the $y(\mathbf{x})$ as posterior probabilities.

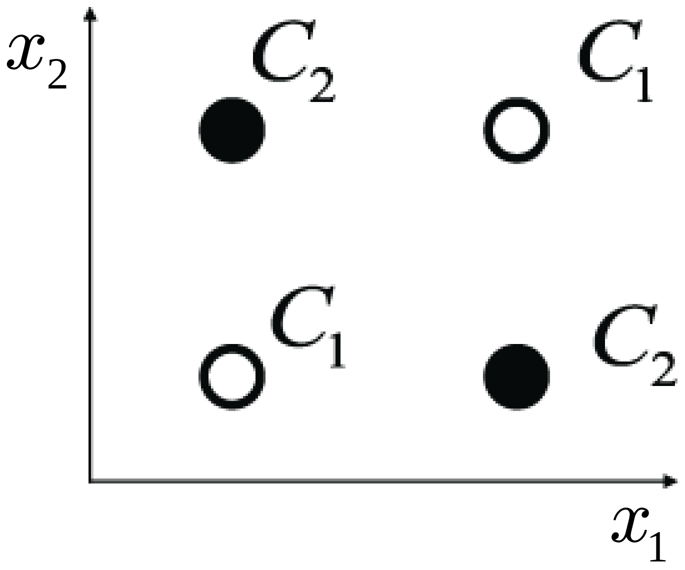


$$g(a) \equiv \frac{1}{1 + \exp(-a)}$$

Recap: Linear Separability

- Up to now: restrictive assumption
  - Only consider linear decision boundaries

- Classical counterexample: XOR



Recap: Extension to Nonlinear Basis Fcts.

- Generalization
  - Transform vector $\mathbf{x}$ with M nonlinear basis functions $\phi_j(\mathbf{x})$:

$$y_k(\mathbf{x}) = \sum_{j=1}^{M} w_{ki}\phi_j(\mathbf{x}) + w_{k0}$$

- Advantages
  - Transformation allows non-linear decision boundaries.
  - By choosing the right ϕ_j, every continuous function can (in principle) be approximated with arbitrary accuracy.
- Disadvatage
  - The error function can in general no longer be minimized in closed form.

  $\Rightarrow$ Minimization with Gradient Descent

Recap: Probabilistic Discriminative Models

- Consider models of the form

$$p(\mathcal{C}_1|\phi) = y(\phi) = \sigma(\mathrm{w}^T\phi)$$

with

$$p(\mathcal{C}_2|\phi) = 1 - p(\mathcal{C}_1|\phi)$$

- This model is called logistic regression.

- Properties
  - Probabilistic interpretation
  - But discriminative method: only focus on decision hyperplane
  - Advantageous for high-dimensional spaces, requires less parameters than explicitly modeling $p(\phi|\mathcal{C}_k)$ and $p(\mathcal{C}_k)$.

Recap: Logistic Regression

- Let's consider a data set $\{\phi_n, t_n\}$ with $n = 1,\ldots,N$, where $\phi_n = \phi(\mathbf{x}_n)$ and $t_n \in \{0,1\}$ $\mathbf{t} = (t_1, \ldots, t_N)^T$

- With $y_n = p(\mathcal{C}_1|\phi_n)$, we can write the likelihood as

$$p(\mathbf{t}|\mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n} \{1 - y_n\}^{1-t_n}$$

- Define the error function as the negative log-likelihood

$$\begin{aligned} E(\mathbf{w}) &= -\ln p(\mathbf{t}|\mathbf{w}) \\ &= -\sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\} \end{aligned}$$

  - This is the so-called cross-entropy error function.

Recap: Iterative Methods for Estimation

- Gradient Descent (1st order)

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \, \nabla E(\mathbf{w})\big|_{\mathbf{w}^{(\tau)}}$$

  - Simple and general
  - Relatively slow to converge, has problems with some functions

- Newton-Raphson (2nd order)

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \, \mathbf{H}^{-1} \nabla E(\mathbf{w})\big|_{\mathbf{w}^{(\tau)}}$$

  where $\mathbf{H} = \nabla\nabla E(\mathbf{w})$ is the Hessian matrix, i.e. the matrix of second derivatives.

  - Local quadratic approximation to the target function
  - Faster convergence

Recap: Iteratively Reweighted Least Squares

- Update equations

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - (\mathbf{\Phi}^T\mathbf{R}\mathbf{\Phi})^{-1}\mathbf{\Phi}^T(\mathbf{y}-\mathbf{t})$$

$$= (\mathbf{\Phi}^T\mathbf{R}\mathbf{\Phi})^{-1}\left\{\mathbf{\Phi}^T\mathbf{R}\mathbf{\Phi}\mathbf{w}^{(\tau)} - \mathbf{\Phi}^T(\mathbf{y}-\mathbf{t})\right\}$$

$$= (\mathbf{\Phi}^T\mathbf{R}\mathbf{\Phi})^{-1}\mathbf{\Phi}^T\mathbf{R}\mathbf{z}$$

with $\mathbf{z} = \mathbf{\Phi}\mathbf{w}^{(\tau)} - \mathbf{R}^{-1}(\mathbf{y}-\mathbf{t})$

- Very similar form to pseudo-inverse (normal equations)
  - But now with non-constant weighing matrix $\mathbf{R}$ (depends on $\mathbf{w}$).
  - Need to apply normal equations iteratively.

  $\Rightarrow$ Iteratively Reweighted Least-Squares (IRLS)

Recap: Softmax Regression

- Multi-class generalization of logistic regression
  - In logistic regression, we assumed binary labels $t_n \in \{0, 1\}$
  - Softmax generalizes this to K values in 1-of-K notation.

$$\mathbf{y}(\mathbf{x};\mathbf{w}) = \begin{bmatrix} P(y=1|\mathbf{x};\mathbf{w}) \\ P(y=2|\mathbf{x};\mathbf{w}) \\ \vdots \\ P(y=K|\mathbf{x};\mathbf{w}) \end{bmatrix} = \frac{1}{\sum_{j=1}^{K} \exp(\mathbf{w}_j^\top \mathbf{x})} \begin{bmatrix} \exp(\mathbf{w}_1^\top \mathbf{x}) \\ \exp(\mathbf{w}_2^\top \mathbf{x}) \\ \vdots \\ \exp(\mathbf{w}_K^\top \mathbf{x}) \end{bmatrix}$$

  - This uses the softmax function

$$\frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

  - Note: the resulting distribution is normalized.

Recap: Softmax Regression Cost Function

- Logistic regression
  - Alternative way of writing the cost function

$$\begin{aligned} E(\mathbf{w}) &= -\sum_{n=1}^{N} \{t_n \ln y_n + (1-t_n)\ln(1-y_n)\} \\ &= -\sum_{n=1}^{N}\sum_{k=0}^{1} \{\mathbb{I}\left(t_n = k\right) \ln P\left(y_n = k | \mathbf{x}_n; \mathbf{w}\right)\} \end{aligned}$$

- Softmax regression
  - Generalization to K classes using indicator functions.

$$E(\mathbf{w}) = -\sum_{n=1}^{N}\sum_{k=1}^{K} \left\{ \mathbb{I}\left(t_n = k\right) \ln \frac{\exp(\mathbf{w}_k^\top \mathbf{x})}{\sum_{j=1}^{K} \exp(\mathbf{w}_j^\top \mathbf{x})} \right\}$$

$$\nabla_{\mathbf{w}_k} E(\mathbf{w}) = -\sum_{n=1}^{N} \left[\mathbb{I}\left(t_n = k\right) \ln P\left(y_n = k | \mathbf{x}_n; \mathbf{w}\right)\right]$$

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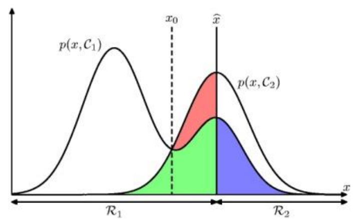
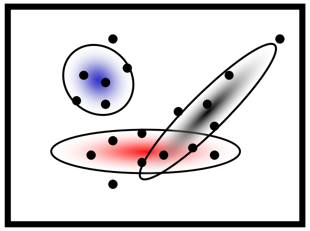
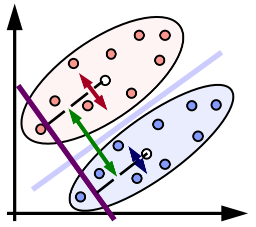
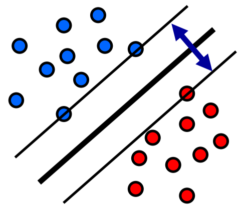
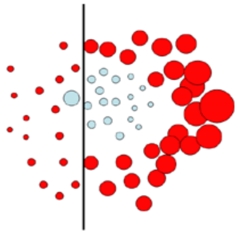
  - Probability Density Estimation
- Classification Approaches
  - Linear Discriminants
  - Support Vector Machines
  - Ensemble Methods & Boosting
- Deep Learning
  - Foundations
  - Convolutional Neural Networks
  - Recurrent Neural Networks

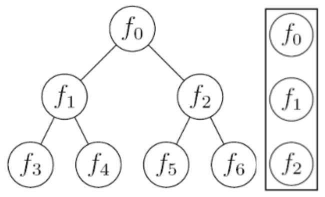


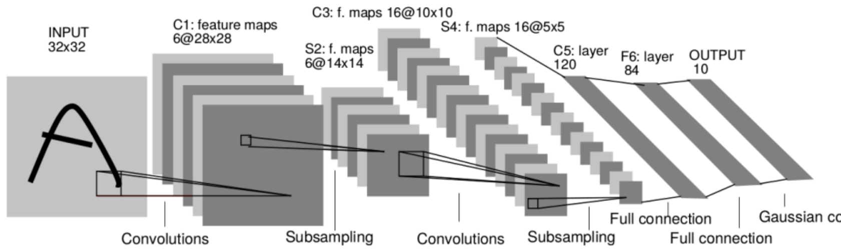




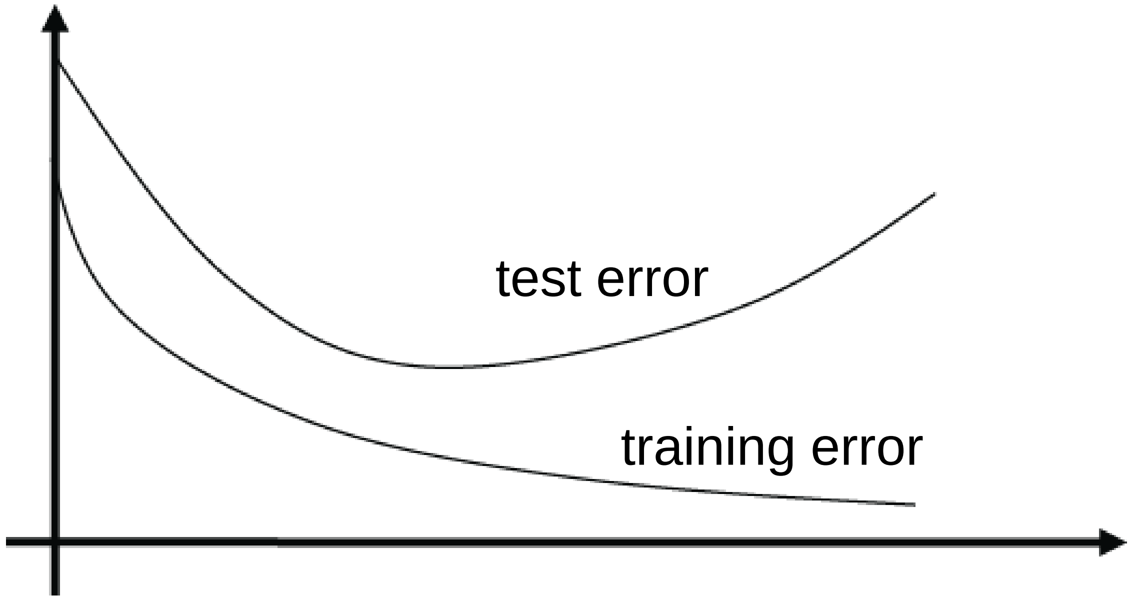








Recap: Generalization and Overfitting



- Goal: predict class labels of new observations
  - Train classification model on limited training set.
  - The further we optimize the model parameters, the more the training error will decrease.
  - However, at some point the test error will go up again.

  $\Rightarrow$ *Overfitting to the training set!*

Image source: B. Schiele

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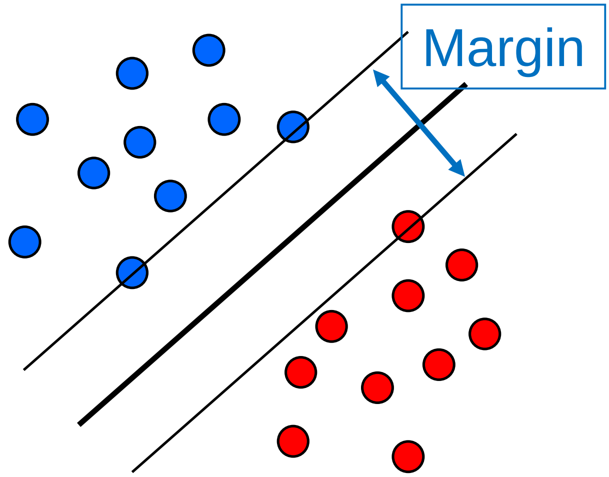
Recap: Support Vector Machine (SVM)

- Basic idea
  - The SVM tries to find a classifier which maximizes the margin between pos. and neg. data points.
  - Up to now: consider linear classifiers

$$\mathbf{w}^{\mathrm{T}}\mathbf{x} + b = 0$$



- Formulation as a convex optimization problem
  - Find the hyperplane satisfying

$$\underset{\mathbf{w},b}{\arg\min}\ \frac{1}{2}\|\mathbf{w}\|^2$$

under the constraints

$$t_n(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b) \geq 1 \quad \forall n$$

based on training data points $\mathbf{x}_n$ and target values $t_n \in \{-1, 1\}$

Recap: SVM – Primal Formulation

- Lagrangian primal form

$$L_p = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n \left\{ t_n(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b) - 1 \right\}$$

$$= \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n \left\{ t_n y(\mathbf{x}_n) - 1 \right\}$$

- The solution of L_p needs to fulfill the KKT conditions
  - Necessary and sufficient conditions

$$\begin{aligned} a_n &\geq 0 \\ t_n y(\mathbf{x}_n) - 1 &\geq 0 \\ a_n \left\{ t_n y(\mathbf{x}_n) - 1 \right\} &= 0 \end{aligned}$$

KKT:

$$\begin{aligned} \lambda &\geq 0 \\ f(\mathbf{x}) &\geq 0 \\ \lambda f(\mathbf{x}) &= 0 \end{aligned}$$

Recap: SVM – Solution

- Solution for the hyperplane
  - Computed as a linear combination of the training examples

$$\mathbf{w} = \sum_{n=1}^{N} a_n t_n \mathbf{x}_n$$

  - Sparse solution: $a_n \neq 0$ only for some points, the support vectors

$\Rightarrow$ Only the SVs actually influence the decision boundary!

  - Compute b by averaging over all support vectors:

$$b = \frac{1}{N_{\mathcal{S}}} \sum_{n \in \mathcal{S}} \left(t_n - \sum_{m \in \mathcal{S}} a_m t_m \mathbf{x}_m^{\mathrm{T}} \mathbf{x}_n \right)$$

Recap: SVM – Support Vectors

- The training points for which $a_n > 0$ are called "support vectors".
- Graphical interpretation:
  - The support vectors are the points on the margin.
  - They *define* the margin and thus the hyperplane.

$\Rightarrow$ All other data points can be discarded!

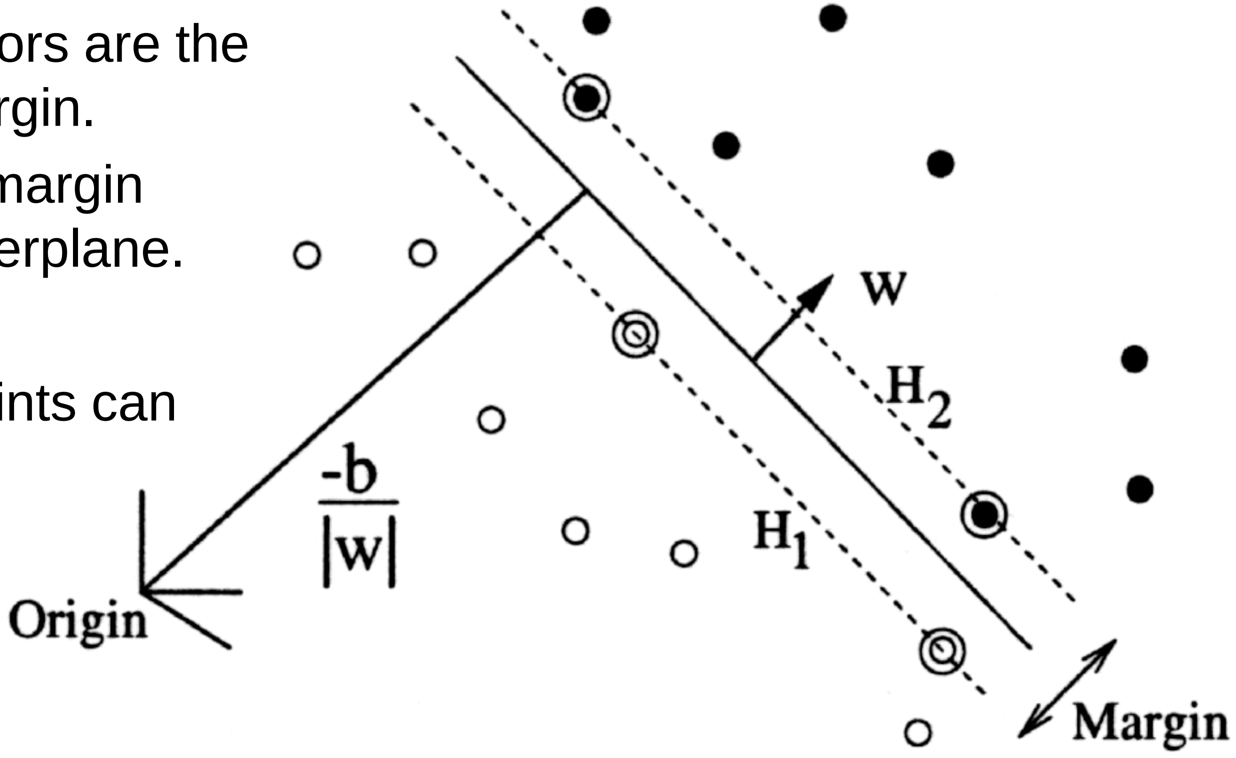


Image source: C. Burges, 1998

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Recap: SVM – Dual Formulation

see Exercise 2.2

- Maximize

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m (\mathbf{x}_m^{\mathrm{T}} \mathbf{x}_n)$$

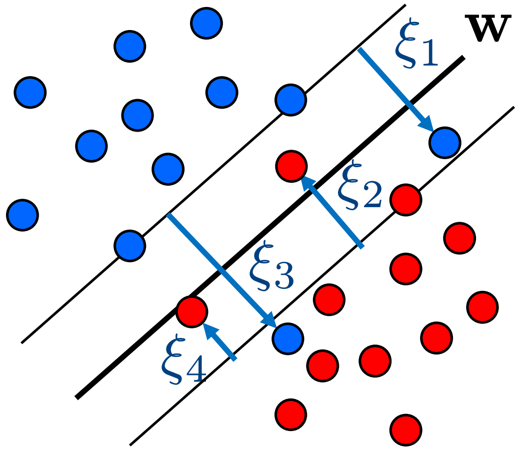
under the conditions

$$\begin{aligned} a_n &\geq 0 \quad \forall n \\ \sum_{n=1}^{N} a_n t_n &= 0 \end{aligned}$$

- Comparison
  - L_d is equivalent to the primal form L_p, but only depends on a_n.
  - L_p scales with $\mathcal{O}(D^3)$.
  - L_d scales with $\mathcal{O}(N^3)$ – in practice between $\mathcal{O}(N)$ and $\mathcal{O}(N^2)$.

Recap: SVM for Non-Separable Data

- Slack variables
  - One slack variable $\xi_n \geq 0$ for each training data point.
- Interpretation
  - $\xi_n = 0$ for points that are on the correct side of the margin.
  - $\xi_n = |t_n - y(\mathbf{x}_n)|$ for all other points.



Point on decision boundary: $\xi_n = 1$

Misclassified point: $\xi_n > 1$

- We do not have to set the slack variables ourselves!

$\Rightarrow$ They are jointly optimized together with $\mathbf{w}$.

Recap: SVM – New Dual Formulation

see Exercise 2.2

- New SVM Dual: Maximize

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m (\mathbf{x}_m^{\mathrm{T}}\mathbf{x}_n)$$

under the conditions

$$0 \cdot \quad a_n \cdot \quad C$$

$$\sum_{n=1}^{N} a_n t_n \quad = \quad 0$$

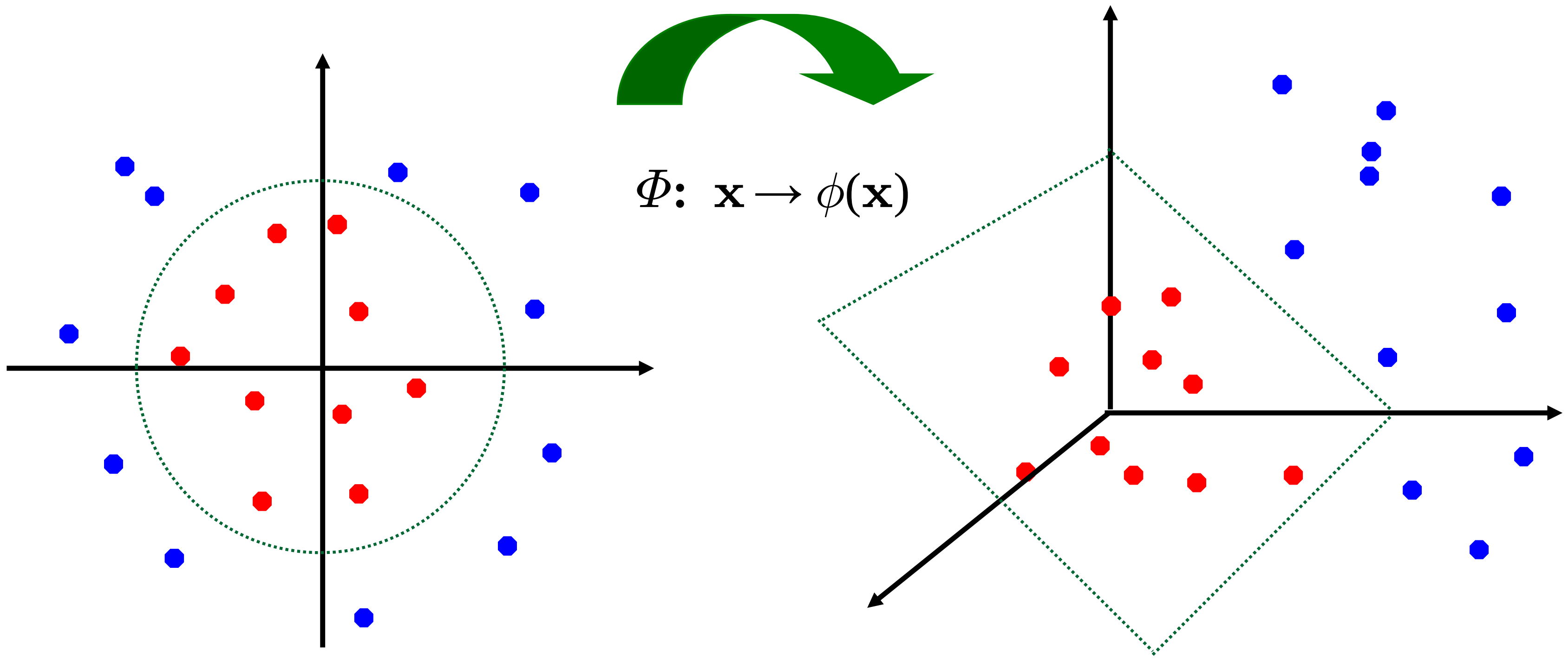
This is all that changed!

- This is again a quadratic programming problem

  $\Rightarrow$ Solve as before…

Recap: Nonlinear SVMs

- General idea: The original input space can be mapped to some higher-dimensional feature space where the training set is separable:



Slide credit: Raymond Mooney

Recap: The Kernel Trick

- Important observation
  - $\phi(\mathbf{x})$ only appears in the form of dot products $\phi(\mathbf{x})^{\mathrm{T}}\phi(\mathbf{y})$:

$$\begin{aligned} y(\mathbf{x}) &= \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + b \\ &= \sum_{n=1}^{N} a_n t_n \phi(\mathbf{x}_n)^{\mathrm{T}}\phi(\mathbf{x}) + b \end{aligned}$$

  - Define a so-called kernel function $k(\mathbf{x},\mathbf{y}) = \phi(\mathbf{x})^{\mathrm{T}}\phi(\mathbf{y})$.
  - Now, in place of the dot product, use the kernel instead:

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}_n, \mathbf{x}) + b$$

  - The kernel function *implicitly* maps the data to the higher-dimensional space (without having to compute $\phi(\mathbf{x})$ explicitly)!

Recap: Kernels Fulfilling Mercer's Condition

- Polynomial kernel

$$k(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^{\mathrm{T}}\mathbf{y} + 1)^p$$

- Radial Basis Function kernel

$$k(\mathbf{x}, \mathbf{y}) = \exp\left\{-\frac{(\mathbf{x} - \mathbf{y})^2}{2\sigma^2}\right\}$$

e.g. Gaussian

- Hyperbolic tangent kernel

$$k(\mathbf{x}, \mathbf{y}) = \tanh(\kappa\mathbf{x}^{\mathrm{T}}\mathbf{y} + \delta)$$

e.g. Sigmoid

  - And many, many more, including kernels on graphs, strings, and symbolic data…

Recap: Kernels Fulfilling Mercer's Condition

- Polynomial kernel

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e.g. Gaussian

- Hyperbolic tangent kernel

$$k(\mathbf{x},\mathbf{y}) = \cancel{\tanh(\kappa\mathbf{x}^{\mathrm{T}}\mathbf{y}+\delta)}$$

e.g. Sigmoid

Actually, that was wrong in the original SVM paper...

  - And many, many more, including kernels on graphs, strings, and symbolic data…

Recap: Nonlinear SVM – Dual Formulation

see Exercise 2.2

- SVM Dual: Maximize

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_m, \mathbf{x}_n)$$

under the conditions

$$0 \cdot \quad a_n \cdot \quad C$$

$$\sum_{n=1}^{N} a_n t_n \quad = \quad 0$$

- Classify new data points using

$$y(\mathbf{x}) \quad = \quad \sum_{n=1}^{N} a_n t_n k(\mathbf{x}_n, \mathbf{x}) + b$$

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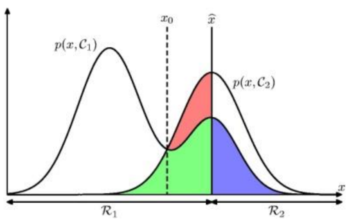
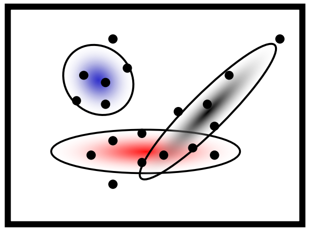
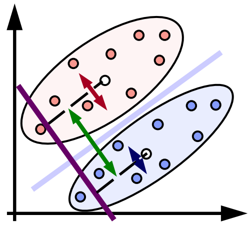
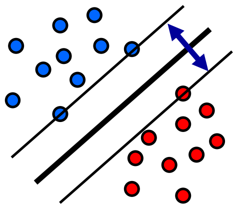
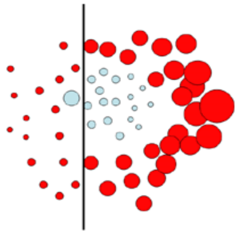
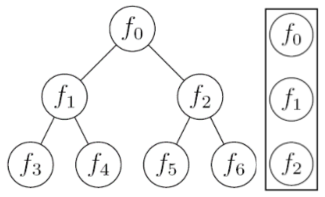


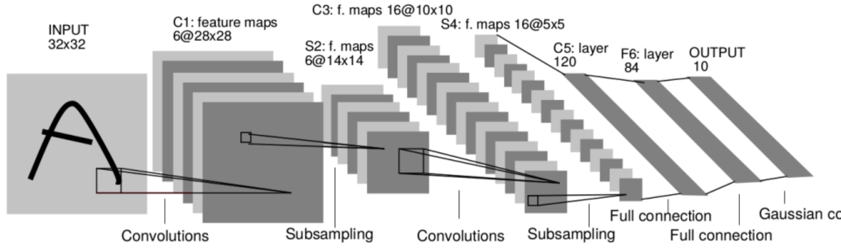






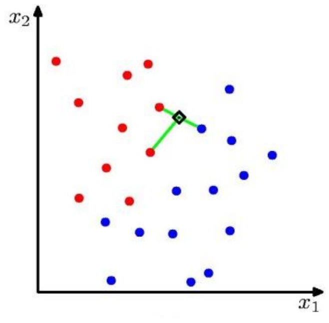


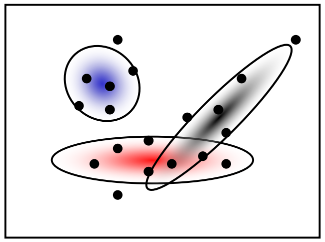


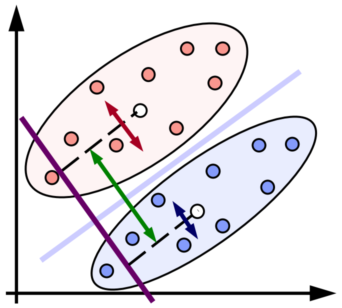


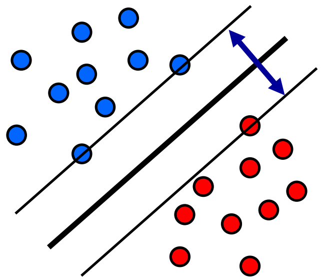
Recap: Classifier Combination

- We've seen already a variety of different classifiers
  - k-NN
  - Bayes classifiers
  - Fisher's Linear Discriminant
  - SVMs









- Each of them has their strengths and weaknesses…
  - Can we improve performance by combining them?

Recap: Bayesian Model Averaging

- Model Averaging
  - Suppose we have H different models $h = 1,\ldots,H$ with prior probabilities $p(h)$.
  - Construct the marginal distribution over the data set

$$p(\mathbf{X}) = \sum_{h=1}^{H} p(\mathbf{X}|h)p(h)$$

- Average error of committee

$$\mathbb{E}_{COM} = \frac{1}{M}\mathbb{E}_{AV}$$

  - This suggests that the average error of a model can be reduced by a factor of M simply by averaging M versions of the model!
  - Unfortunately, this assumes that the errors are all uncorrelated. In practice, they will typically be highly correlated.

Recap: AdaBoost – "Adaptive Boosting"

- Main idea [Freund & Schapire, 1996]
  - Instead of resampling, reweight misclassified training examples.
    - Increase the chance of being selected in a sampled training set.
    - Or increase the misclassification cost when training on the full set.

- Components
  - $h_m(\mathbf{x})$: "weak" or base classifier
    - Condition: <50% training error over any distribution
  - $H(\mathbf{x})$: "strong" or final classifier

- AdaBoost:
  - Construct a strong classifier as a thresholded linear combination of the weighted weak classifiers:

$$H(\mathbf{x}) = sign\left(\sum_{m=1}^{M} \alpha_m h_m(\mathbf{x})\right)$$

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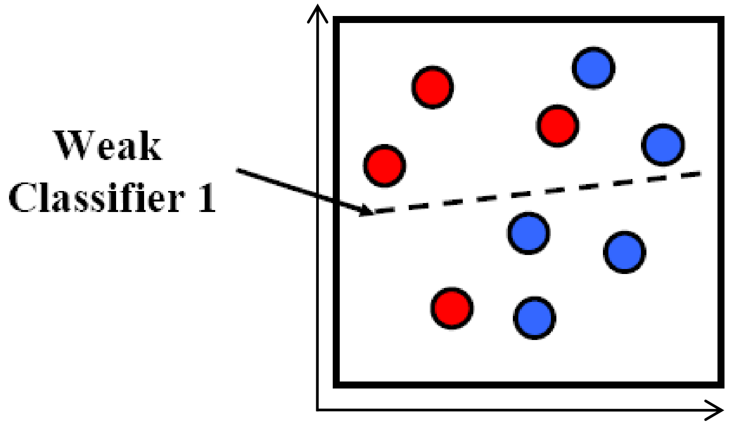
Recap: AdaBoost – Intuition

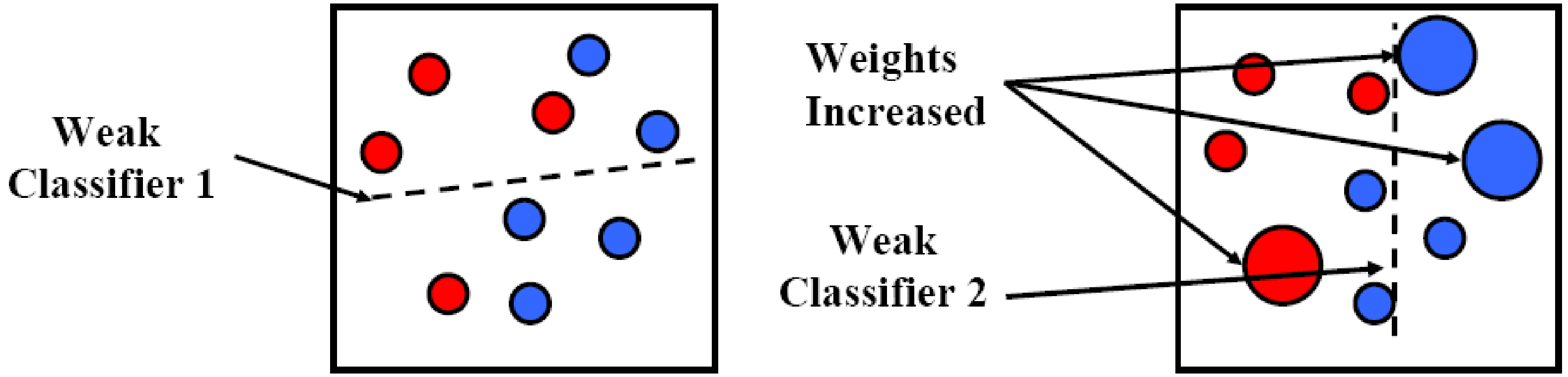


Consider a 2D feature space with positive and negative examples.

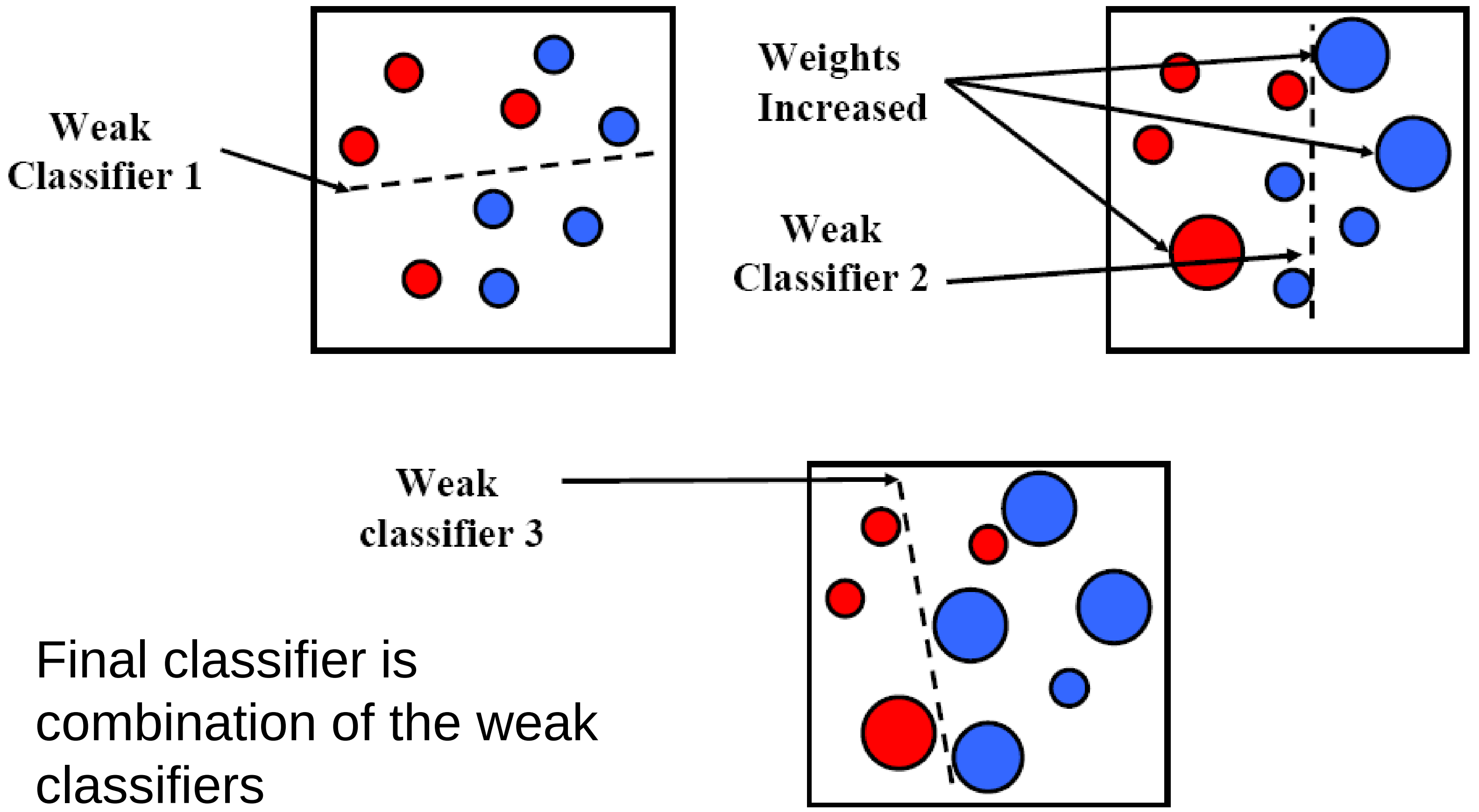
Each weak classifier splits the training examples with at least 50% accuracy.

Examples misclassified by a previous weak learner are given more emphasis at future rounds.

Recap: AdaBoost – Intuition



Recap: AdaBoost – Intuition



Final classifier is combination of the weak classifiers

Recap: AdaBoost – Algorithm

see Exercise 3.1

1. Initialization: Set $w_n^{(1)} = \frac{1}{N}$ for $n = 1,\ldots,N$.
2. For $m = 1,\ldots,M$ iterations
   a) Train a new weak classifier $h_m(\mathbf{x})$ using the current weighting coefficients $\mathbf{W}^{(m)}$ by minimizing the weighted error function

   $$J_m = \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n)$$

   $$I(A) = \begin{cases} 1, & \text{if } A \text{ is true} \\ 0, & \text{else} \end{cases}$$

   b) Estimate the weighted error of this classifier on $\mathbf{X}$:

   $$\epsilon_m = \frac{\sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n)}{\sum_{n=1}^{N} w_n^{(m)}}$$

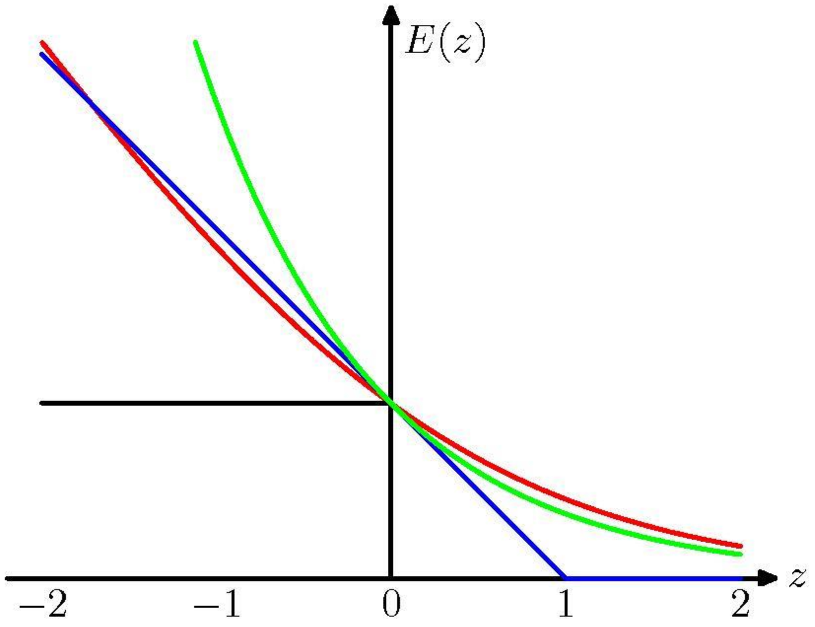
   c) Calculate a weighting coefficient for $h_m(\mathbf{x})$:

   $$\alpha_m = \ln\left\{\frac{1-\epsilon_m}{\epsilon_m}\right\}$$

   d) Update the weighting coefficients:

   $$w_n^{(m+1)} = w_n^{(m)} \exp\left\{\alpha_m I(h_m(\mathbf{x}_n) \neq t_n)\right\}$$

Recap: Comparing Error Functions

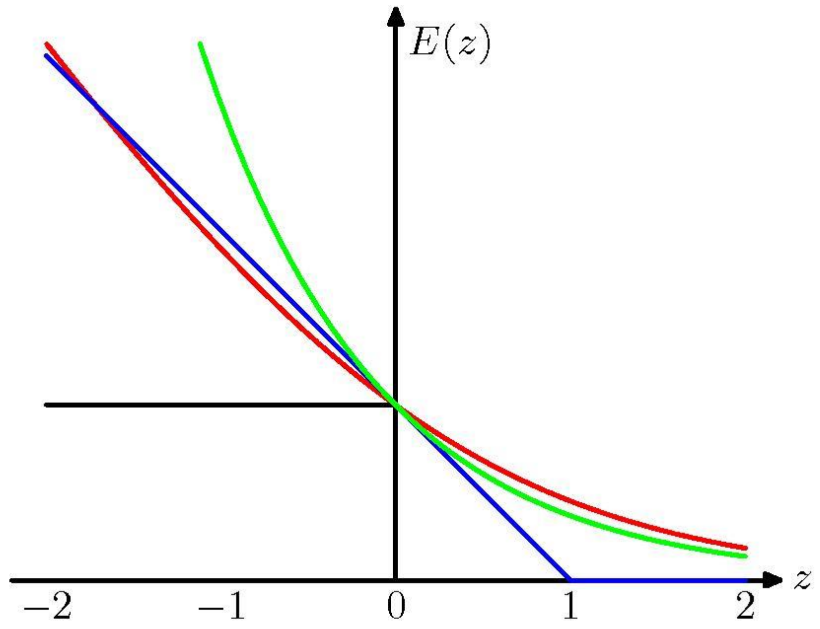


- Ideal misclassification error function
- "Hinge error" used in SVMs
- Exponential error function
  - Continuous approximation to ideal misclassification function.
  - Sequential minimization leads to simple AdaBoost scheme.
  - Disadvantage: exponential penalty for large negative values!

  $\Rightarrow$ Less robust to outliers or misclassified data points!

Image source: Bishop, 2006

Recap: Comparing Error Functions



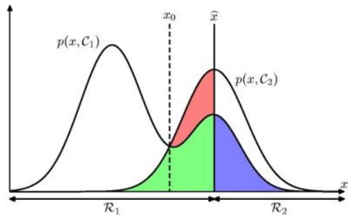
- Ideal misclassification error function
- "Hinge error" used in SVMs
- Exponential error function
- "Cross-entropy error" $E = -\sum \{t_n \ln y_n + (1-t_n)\ln(1-y_n)\}$
  - Similar to exponential error for z>0.
  - Only grows linearly with large negative values of z.

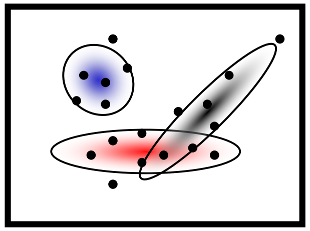
  $\Rightarrow$ Make AdaBoost more robust by switching $\Rightarrow$ "GentleBoost"

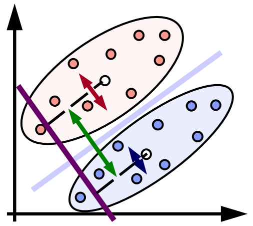
Image source: Bishop, 2006

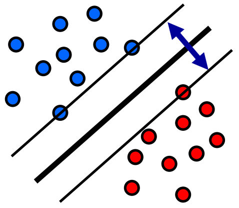
Course Outline

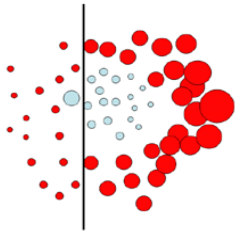
- Fundamentals
  - Bayes Decision Theory
  - Probability Density Estimation
- Classification Approaches
  - Linear Discriminants
  - Support Vector Machines
  - Ensemble Methods & Boosting
- Deep Learning
  - Foundations
  - Convolutional Neural Networks
  - Recurrent Neural Networks

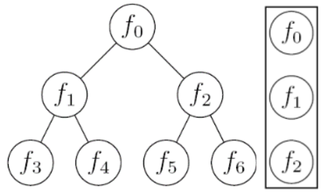


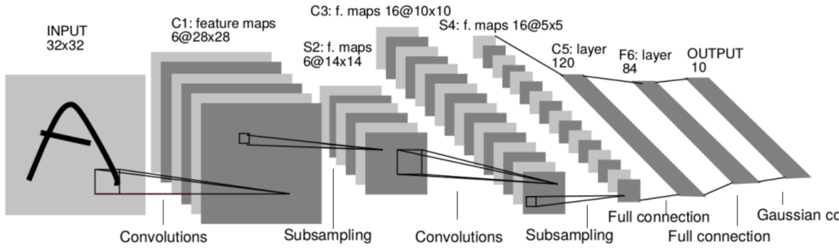






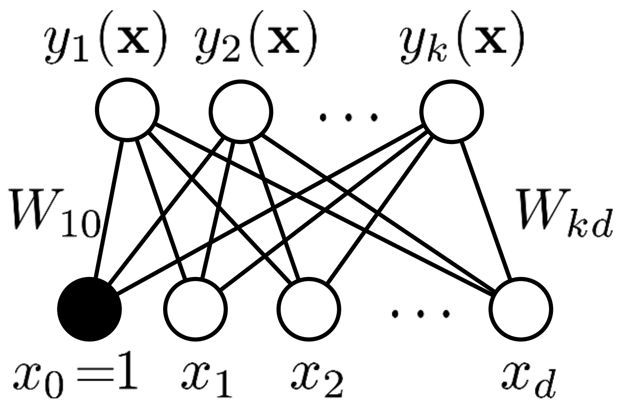






Recap: Perceptrons

- One output node per class


$y_1(\mathbf{x})$ $y_2(\mathbf{x})$ $y_k(\mathbf{x})$
W_{10}
W_{kd}
$x_0 = 1$ x_1 x_2 x_d

Output layer

Weights

Input layer

- Outputs
  - Linear outputs

$$y_k(\mathbf{x}) = \sum_{i=0}^{d} W_{ki} x_i$$

With output nonlinearity

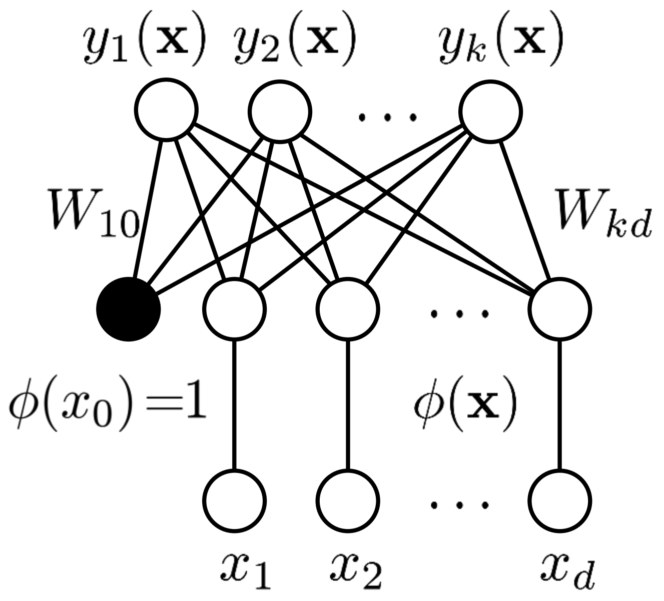
$$y_k(\mathbf{x}) = g\left(\sum_{i=0}^{d} W_{ki} x_i\right)$$

$\Rightarrow$ Can be used to do multidimensional linear regression or multiclass classification.

Slide adapted from Stefan Roth

Recap: Non-Linear Basis Functions

- Straightforward generalization



Output layer

Weights

Feature layer

Mapping (fixed)

Input layer

- Outputs
  - Linear outputs

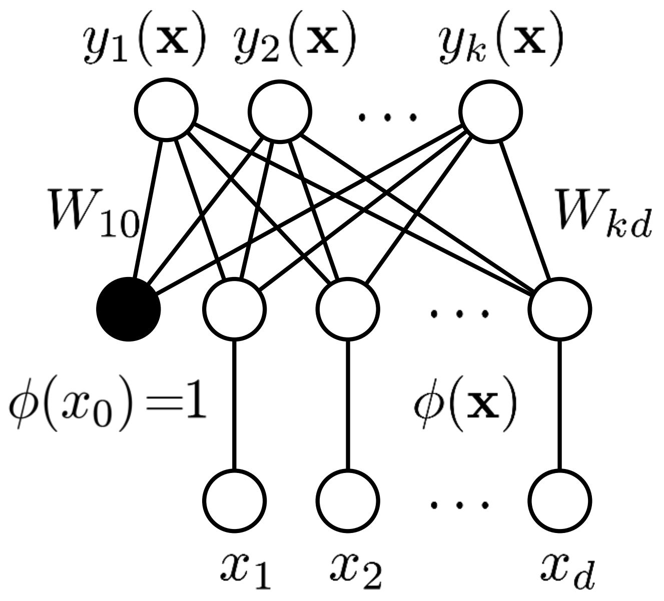
$$y_k(\mathbf{x}) = \sum_{i=0}^{d} W_{ki}\phi(x_i)$$

with output nonlinearity

$$y_k(\mathbf{x}) = g\left(\sum_{i=0}^{d} W_{ki}\phi(x_i)\right)$$

Recap: Non-Linear Basis Functions

- Straightforward generalization



Output layer

Weights

Feature layer

Mapping (fixed)

Input layer

- Remarks
  - Perceptrons are generalized linear discriminants!
  - Everything we know about the latter can also be applied here.
  - Note: feature functions $\phi(\mathbf{x})$ are kept fixed, not learned!

Recap: Perceptron Learning

- Process the training cases in some permutation
  - If the output unit is correct, leave the weights alone.
  - If the output unit incorrectly outputs a zero, add the input vector to the weight vector.
  - If the output unit incorrectly outputs a one, subtract the input vector from the weight vector.

- Translation

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left(y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn} \right) \phi_j(\mathbf{x}_n)$$

  - This is the Delta rule a.k.a. LMS rule!

  $\Rightarrow$ Perceptron Learning corresponds to 1st-order (stochastic) Gradient Descent of a quadratic error function!

Recap: Loss Functions

- We can now also apply other loss functions
  - L$_2$ loss $\Rightarrow$ Least-squares regression

    $$L(t, y(\mathbf{x})) = \sum_n (y(\mathbf{x}_n) - t_n)^2$$

  - L$_1$ loss: $\Rightarrow$ Median regression

    $$L(t, y(\mathbf{x})) = \sum_n |y(\mathbf{x}_n) - t_n|$$

  - Cross-entropy loss $\Rightarrow$ Logistic regression

    $$L(t, y(\mathbf{x})) = -\sum_n \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

  - Hinge loss $\Rightarrow$ SVM classification

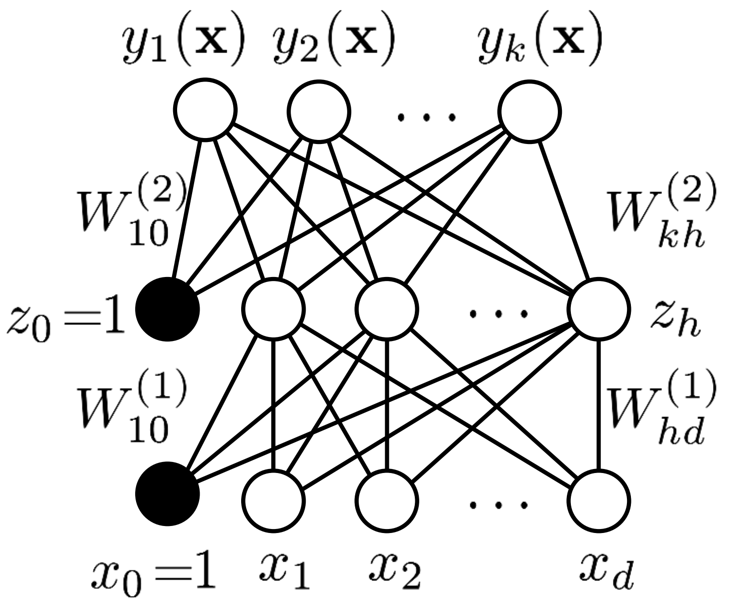
    $$L(t, y(\mathbf{x})) = \sum_n [1 - t_n y(\mathbf{x}_n)]_+$$

  - Softmax loss $\Rightarrow$ Multi-class probabilistic classification

    $$L(t, y(\mathbf{x})) = -\sum_n \sum_k \left\{ \mathbb{I}(t_n = k) \ln \frac{\exp(y_k(\mathbf{x}))}{\sum_j \exp(y_j(\mathbf{x}))} \right\}$$

Recap: Multi-Layer Perceptrons

- Adding more layers



Output layer

Hidden layer

Input layer

- Output

$$y_k(\mathbf{x}) = g^{(2)}\left(\sum_{i=0}^{h} W_{ki}^{(2)} g^{(1)}\left(\sum_{j=0}^{d} W_{ij}^{(1)} x_j\right)\right)$$

Slide adapted from Stefan Roth

Recap: Learning with Hidden Units

- How can we train multi-layer networks efficiently?
  - Need an efficient way of adapting all weights, not just the last layer.

- Idea: Gradient Descent
  - Set up an error function

$$E(\mathbf{W}) = \sum_n L(t_n, y(\mathbf{x}_n; \mathbf{W})) + \lambda\Omega(\mathbf{W})$$

with a loss $L(\cdot)$ and a regularizer $\Omega(\cdot)$.

  - E.g., $L(t, y(\mathbf{x}; \mathbf{W})) = \sum_n \left(y(\mathbf{x}_n; \mathbf{W}) - t_n\right)^2$ L$_2$ loss

$$\Omega(\mathbf{W}) = ||\mathbf{W}||_F^2$$

L$_2$ regularizer ("weight decay")

$\Rightarrow$ Update each weight $W_{ij}^{(k)}$ in the direction of the gradient $\frac{\partial E(\mathbf{W})}{\partial W_{ij}^{(k)}}$

Recap: Gradient Descent

- Two main steps
  1. Computing the gradients for each weight
  2. Adjusting the weights in the direction of the gradient

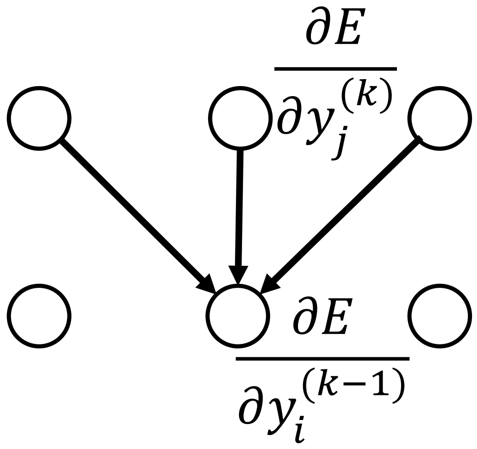
- We consider those two steps separately
  - Computing the gradients: Backpropagation
  - Adjusting the weights: Optimization techniques

Recap: Backpropagation Algorithm

- Core steps
  1. Convert the discrepancy between each output and its target value into an error derivate.
  2. Compute error derivatives in each hidden layer from error derivatives in the layer above.
  3. Use error derivatives *w.r.t.* activities to get error derivatives *w.r.t.* the incoming weights

$$E = \frac{1}{2}\sum_{j \in output}(t_j - y_j)^2$$

$$\frac{\partial E}{\partial y_j} = -(t_j - y_j)$$

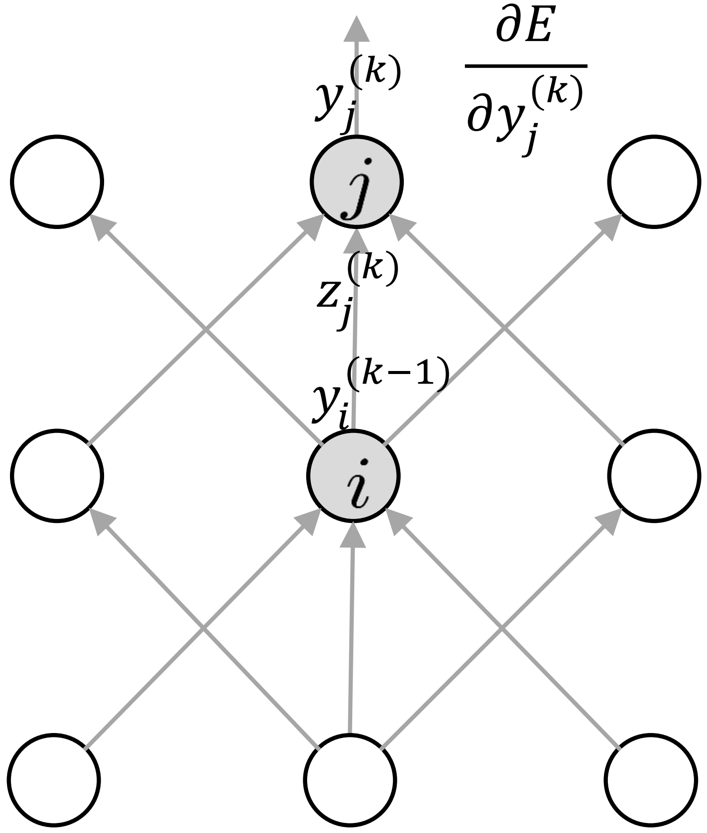


$$\frac{\partial E}{\partial y_j^{(k)}}$$

$$\frac{\partial E}{\partial y_i^{(k-1)}}$$

$$\frac{\partial E}{\partial y_j^{(k)}} \longrightarrow \frac{\partial E}{\partial w_{ji}^{(k-1)}}$$

Recap: Backpropagation Algorithm



$$\frac{\partial E}{\partial z_j^{(k)}} = \frac{\partial y_j^{(k)}}{\partial z_j^{(k)}} \frac{\partial E}{\partial y_j^{(k)}} = \frac{\partial g\left(z_j^{(k)}\right)}{\partial z_j^{(k)}} \frac{\partial E}{\partial y_j^{(k)}}$$

$$\frac{\partial E}{\partial y_i^{(k-1)}} = \sum_j \frac{\partial z_j^{(k)}}{\partial y_i^{(k-1)}} \frac{\partial E}{\partial z_j^{(k)}} = \sum_j w_{ji}^{(k-1)} \frac{\partial E}{\partial z_j^{(k)}}$$

$$\frac{\partial E}{\partial w_{ji}^{(k-1)}} = \frac{\partial z_j^{(k)}}{\partial w_{ji}^{(k-1)}} \frac{\partial E}{\partial z_j^{(k)}} = y_i^{(k-1)} \frac{\partial E}{\partial z_j^{(k)}}$$

- Efficient propagation scheme
  - $y_i^{(k-1)}$ is already known from forward pass! (Dynamic Programming)

$\Rightarrow$ Propagate back the gradient from layer k and multiply with $y_i^{(k-1)}$.

Recap: MLP Backpropagation Algorithm

- Forward Pass

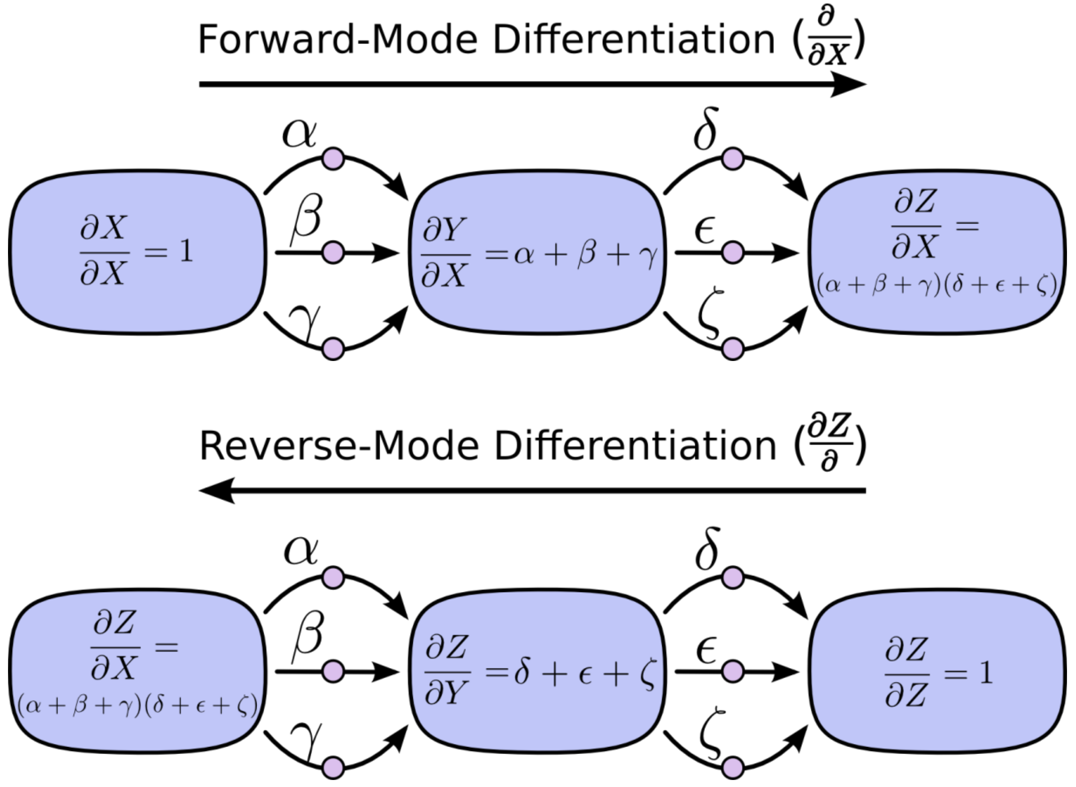
```
$\mathbf{y}^{(0)} = \mathbf{x}$
for $k = 1, ..., l$ do
    $\mathbf{z}^{(k)} = \mathbf{W}^{(k)}\mathbf{y}^{(k-1)}$
    $\mathbf{y}^{(k)} = g_k(\mathbf{z}^{(k)})$
endfor
$\mathbf{y} = \mathbf{y}^{(l)}$
$E = L(\mathbf{t}, \mathbf{y}) + \lambda\Omega(\mathbf{W})$
```

- Backward Pass

```
$\mathbf{h} \leftarrow \frac{\partial E}{\partial \mathbf{y}} = \frac{\partial}{\partial \mathbf{y}} L(\mathbf{t}, \mathbf{y}) + \lambda \frac{\partial}{\partial \mathbf{y}} \Omega$
for $k = l, l\text{-}1, ..., 1$ do
    $\mathbf{h} \leftarrow \frac{\partial E}{\partial \mathbf{z}^{(k)}} = \mathbf{h} \odot g'(\mathbf{y}^{(k)})$
    $\frac{\partial E}{\partial \mathbf{W}^{(k)}} = \mathbf{h}\mathbf{y}^{(k-1)\top} + \lambda \frac{\partial \Omega}{\partial \mathbf{W}^{(k)}}$
    $\mathbf{h} \leftarrow \frac{\partial E}{\partial \mathbf{y}^{(k-1)}} = \mathbf{W}^{(k)\top}\mathbf{h}$
endfor
```

- Notes
  - For efficiency, an entire batch of data $\mathbf{X}$ is processed at once.
  - $\odot$ denotes the element-wise product

Recap: Computational Graphs


Forward-Mode Differentiation ($\frac{\partial}{\partial X}$)
α
β
γ
δ
ϵ
ζ
$\frac{\partial X}{\partial X} = 1$
$\frac{\partial Y}{\partial X} = \alpha + \beta + \gamma$
$\frac{\partial Z}{\partial X} = (\alpha+\beta+\gamma)(\delta+\epsilon+\zeta)$
Reverse-Mode Differentiation ($\frac{\partial Z}{\partial}$)
$\frac{\partial Z}{\partial X} = (\alpha+\beta+\gamma)(\delta+\epsilon+\zeta)$
$\frac{\partial Z}{\partial Y} = \delta + \epsilon + \zeta$
$\frac{\partial Z}{\partial Z} = 1$

Apply operator $\frac{\partial}{\partial X}$ to every node.

Apply operator $\frac{\partial Z}{\partial}$ to every node.

- Forward differentiation needs one pass per node. Reverse-mode differentiation can compute all derivatives in one single pass.

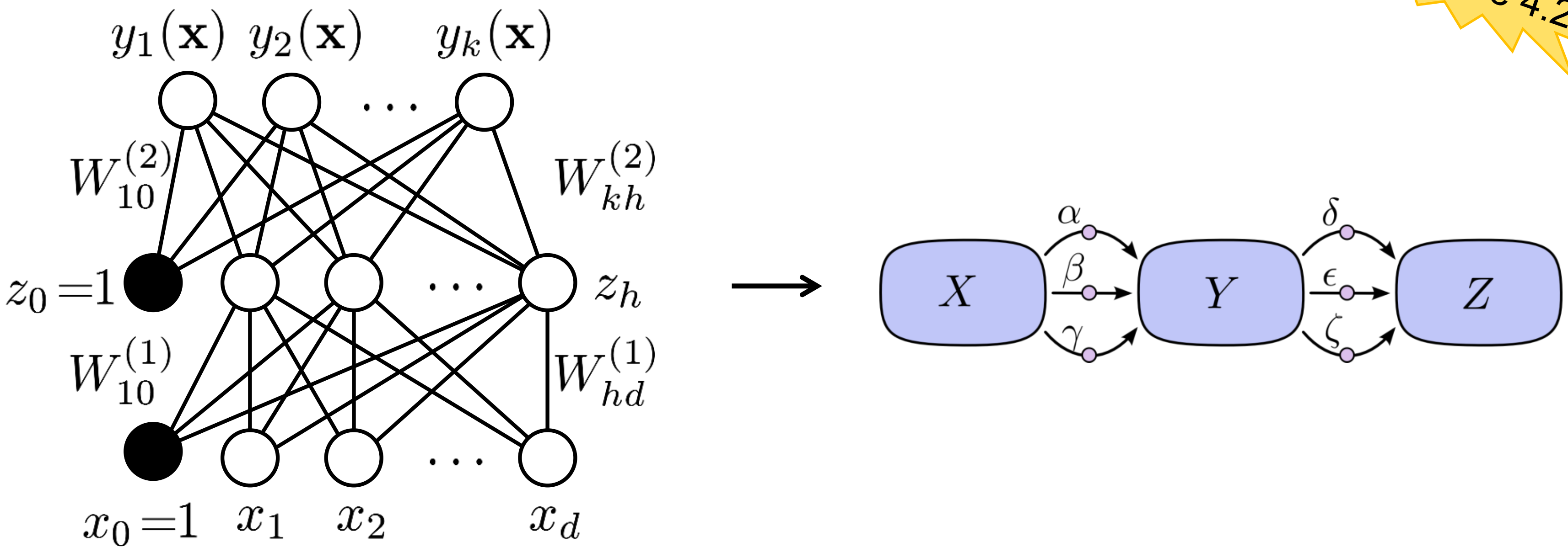
$\Rightarrow$ Speed-up in $\mathcal{O}(\#\text{inputs})$ compared to forward differentiation!

Image source: Christopher Olah, colah.github.io

Recap: Automatic Differentiation

see Exercise 4.2

- Approach for obtaining the gradients



  - Convert the network into a computational graph.
  - Each new layer/module just needs to specify how it affects the forward and backward passes.
  - Apply reverse-mode differentiation.

$\Rightarrow$ Very general algorithm, used in today's Deep Learning packages

Image source: Christopher Olah, colah.github.io

Recap: Choosing the Right Learning Rate

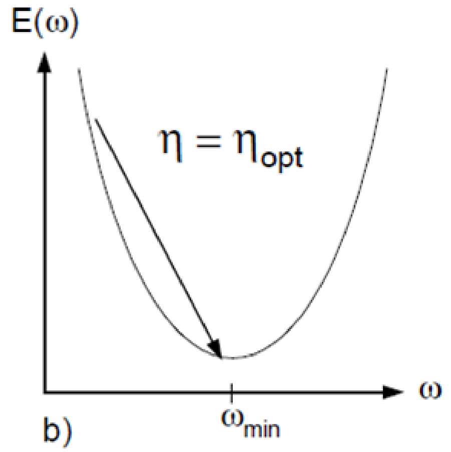
- Convergence of Gradient Descent
  - Simple 1D example

$$W^{(\tau-1)} = W^{(\tau)} - \eta \frac{\mathrm{d}E(W)}{\mathrm{d}W}$$

  - What is the optimal learning rate η_{opt}?
  - If E is quadratic, the optimal learning rate is given by the inverse of the Hessian

$$\eta_{\text{opt}} = \left(\frac{\mathrm{d}^2 E(W^{(\tau)})}{\mathrm{d}W^2} \right)^{-1}$$

  - Advanced optimization techniques try to approximate the Hessian by a simplified form.
  - *If we exceed the optimal learning rate, bad things happen!*



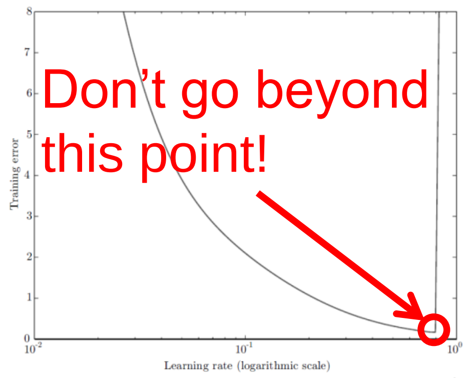
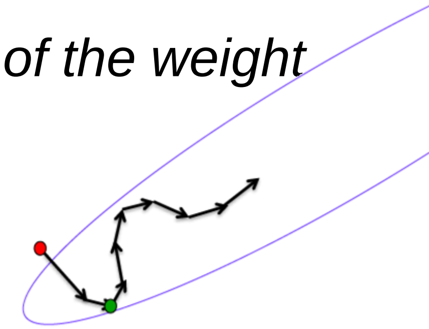


Image source: Yann LeCun et al., Efficient BackProp (1998)

Recap: Advanced Optimization Techniques

- Momentum
  - *Instead of using the gradient to change the position of the weight "particle", use it to change the velocity.*
  - Effect: dampen oscillations in directions of high curvature
  - Nesterov-Momentum: Small variation in the implementation



- RMS-Prop
  - *Separate learning rate for each weight: Divide the gradient by a running average of its recent magnitude.*

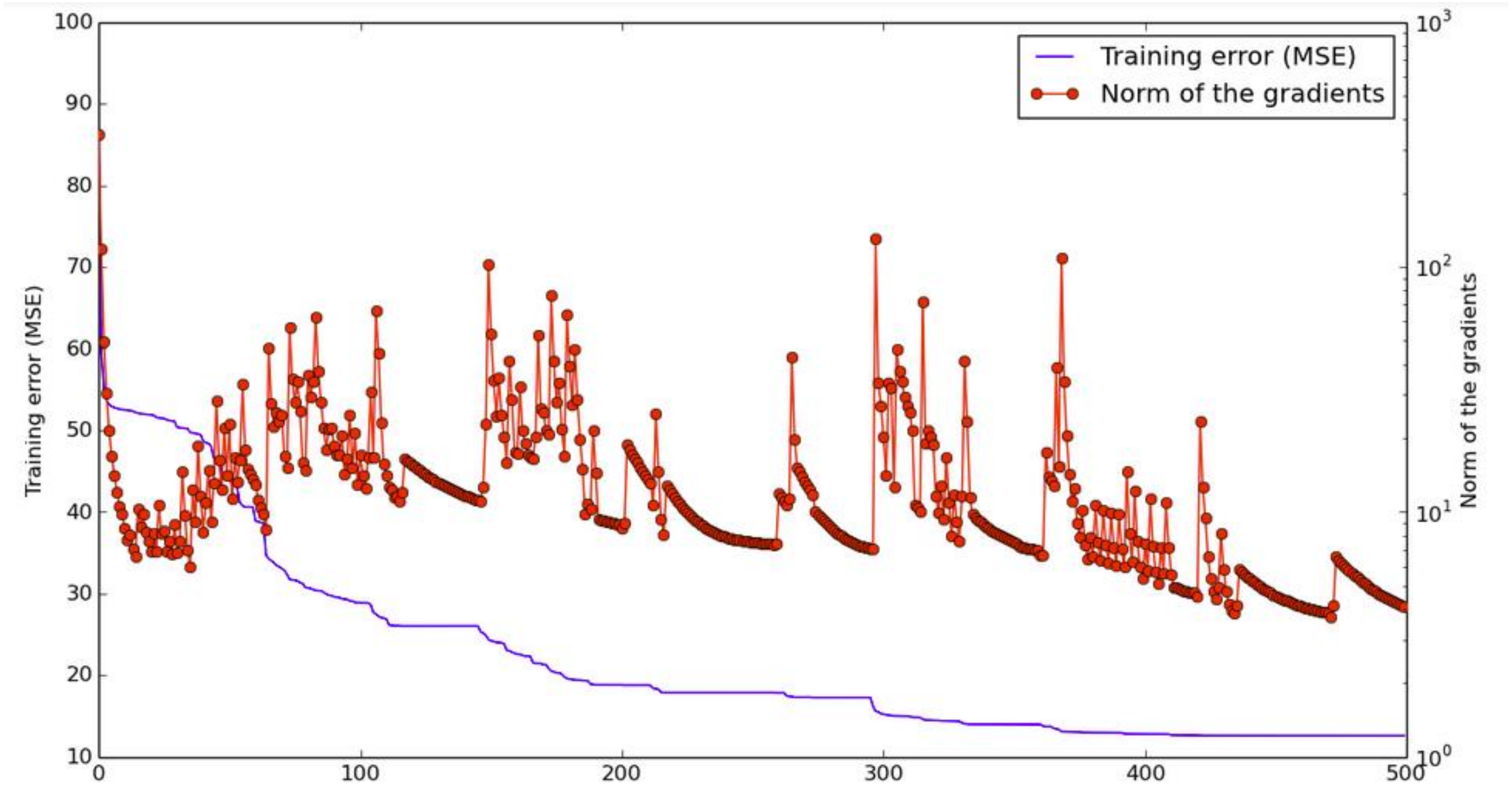
- AdaGrad
- AdaDelta
- Adam

$\left.\vphantom{\begin{matrix}a\\b\\c\end{matrix}}\right\}$ Some more recent techniques, work better for some problems. Try them.

Image source: Geoff Hinton

Recap: Patience

- Saddle points dominate in high-dimensional spaces!

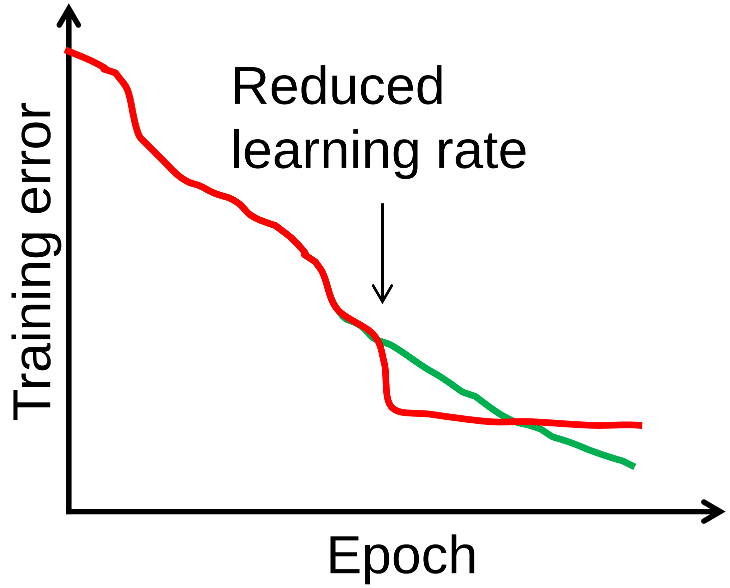


$\Rightarrow$ Learning often doesn’t get stuck, you just may have to wait...

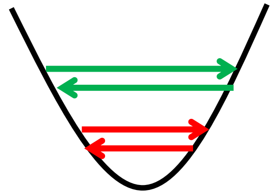
Image source: Yoshua Bengio

Recap: Reducing the Learning Rate

- Final improvement step after convergence is reached
  - Reduce learning rate by a factor of 10.
  - Continue training for a few epochs.
  - Do this 1-3 times, then stop training.



- Effect
  - Turning down the learning rate will reduce the random fluctuations in the error due to different gradients on different minibatches.



- *Be careful: Do not turn down the learning rate too soon!*
  - Further progress will be much slower after that.

Recap: Data Augmentation

- Effect
  - Much larger training set
  - Robustness against expected variations
- During testing
  - When cropping was used during training, need to again apply crops to get same image size.
  - Beneficial to also apply flipping during test.
  - Applying several ColorPCA variations can bring another ~1% improvement, but at a significantly increased runtime.

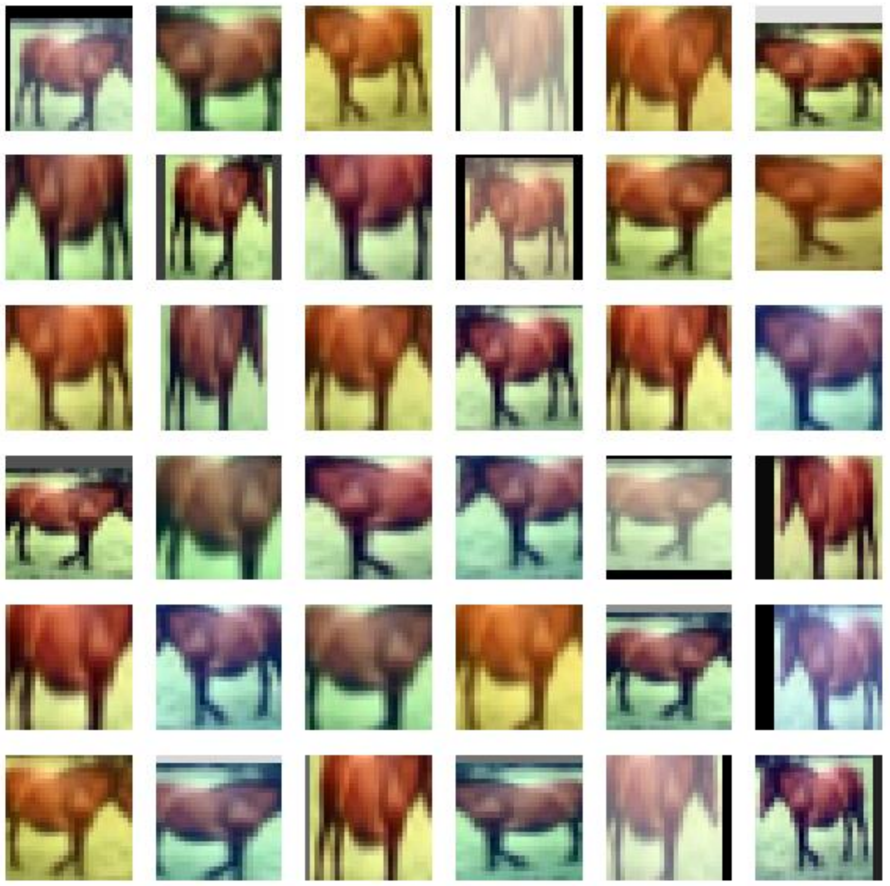
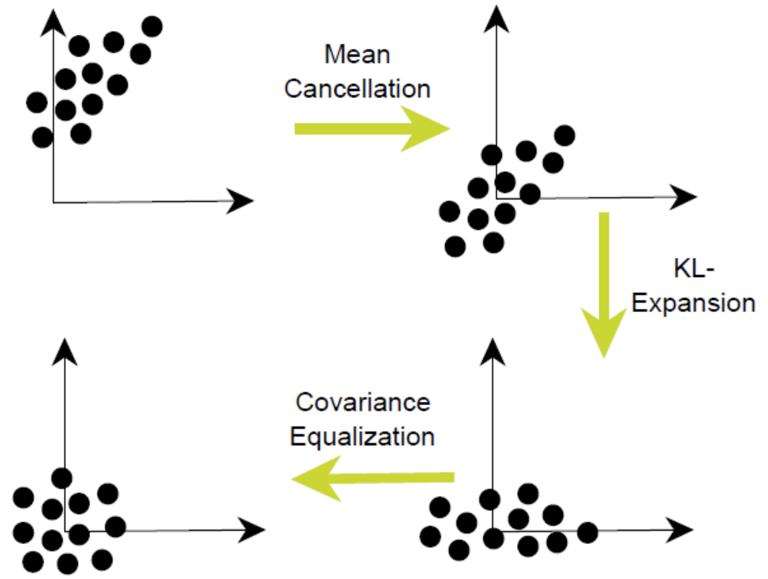

Augmented training data (from one original image)

Image source: Lucas Beyer

Recap: Normalizing the Inputs

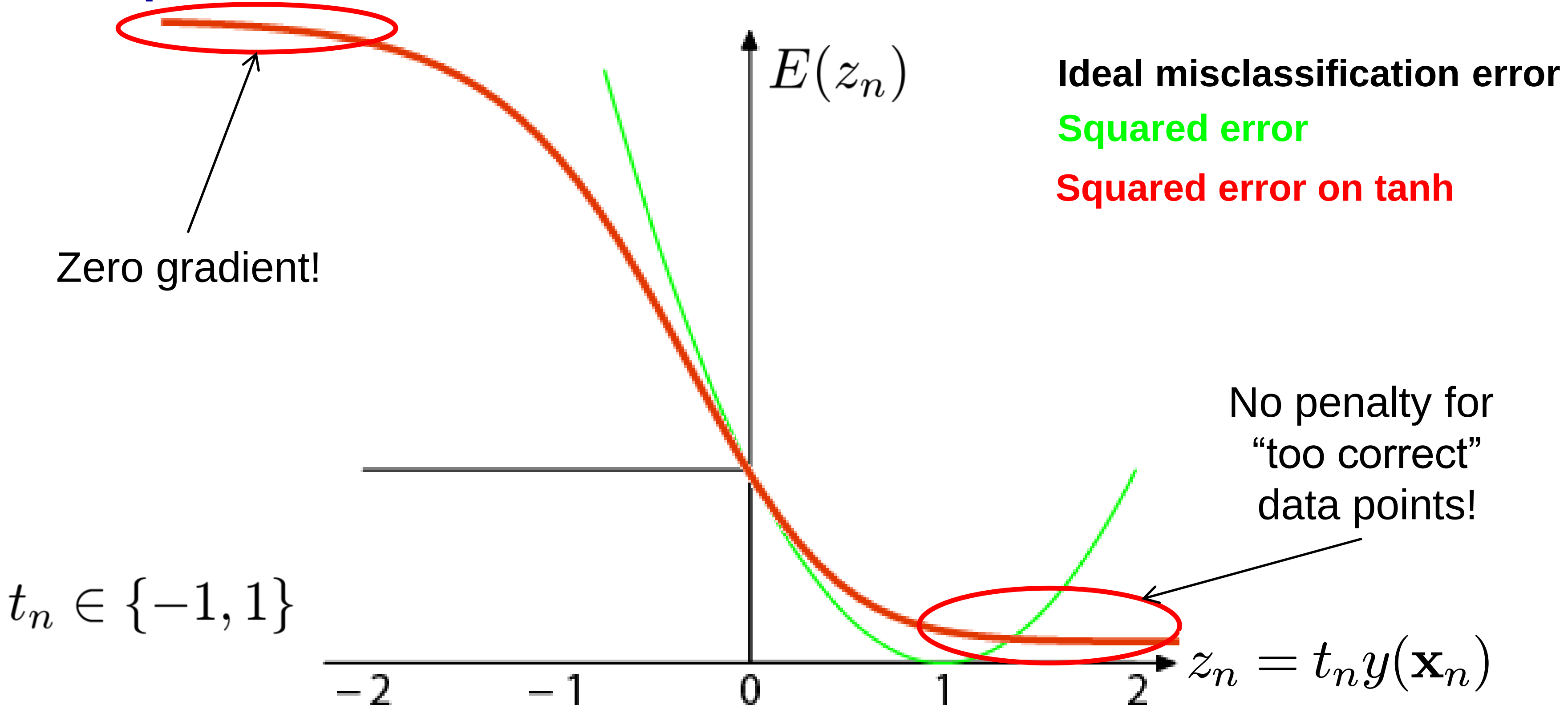
- Convergence is fastest if
  - The mean of each input variable over the training set is zero.
  - The inputs are scaled such that all have the same covariance.
  - Input variables are uncorrelated if possible.



- Advisable normalization steps (for MLPs only, not for CNNs)
  - Normalize all inputs that an input unit sees to zero-mean, unit covariance.
  - If possible, try to decorrelate them using PCA (also known as Karhunen-Loeve expansion).

Image source: Yann LeCun et al., Efficient BackProp (1998)

Recap: Another Note on Error Functions



- Squared error on sigmoid/tanh output function
  - Avoids penalizing "too correct" data points.
  - But: zero gradient for confidently incorrect classifications!

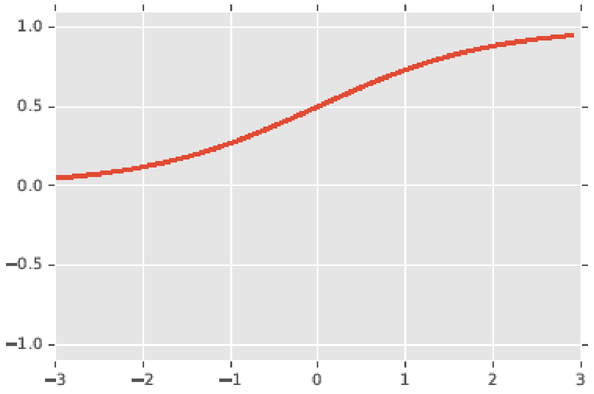
$\Rightarrow$ Do not use L_2 loss with sigmoid outputs (instead: cross-entropy)!

Image source: Bishop, 2006

Recap: Commonly Used Nonlinearities

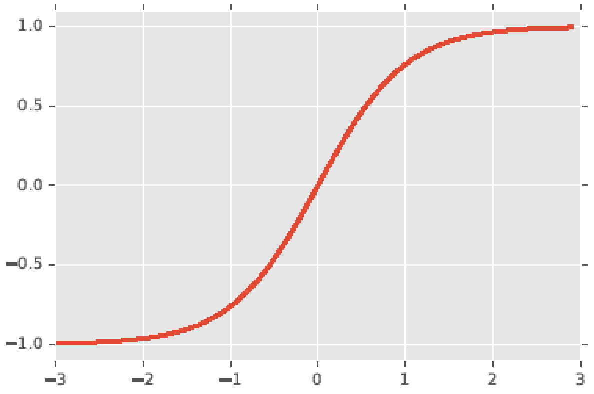
- Sigmoid

$$g(a) = \sigma(a) = \frac{1}{1+\exp\{-a\}}$$



- Hyperbolic tangent

$$g(a) = tanh(a) = 2\sigma(2a) - 1$$



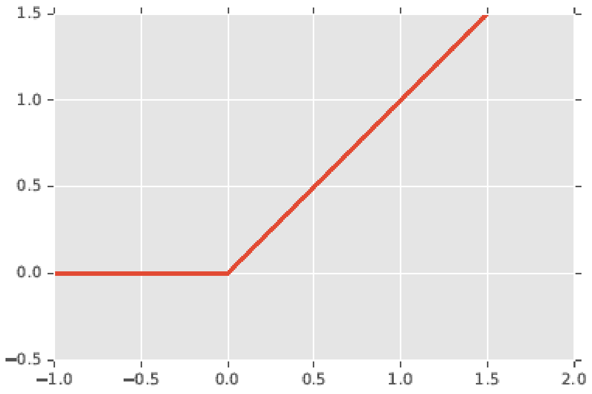
- Softmax

$$g(\mathbf{a}) = \frac{\exp\{-a_i\}}{\sum_j \exp\{-a_j\}}$$

Recap: Commonly Used Nonlinearities (2)

- Rectified linear unit (ReLU)

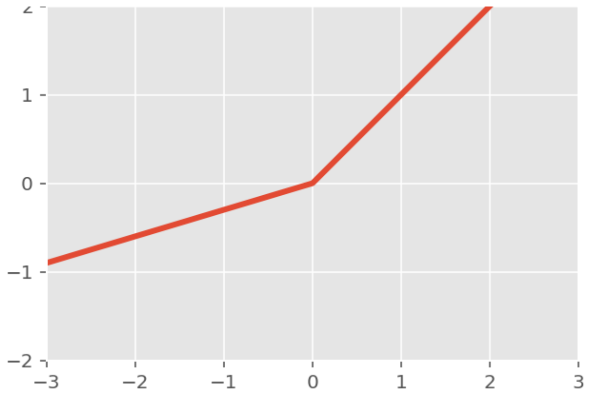
$$g(a) = \max\{0, a\}$$



- Leaky ReLU

$$g(a) = \max\{\beta a, a\} \qquad \beta \in [0.01\,, 0.3]$$

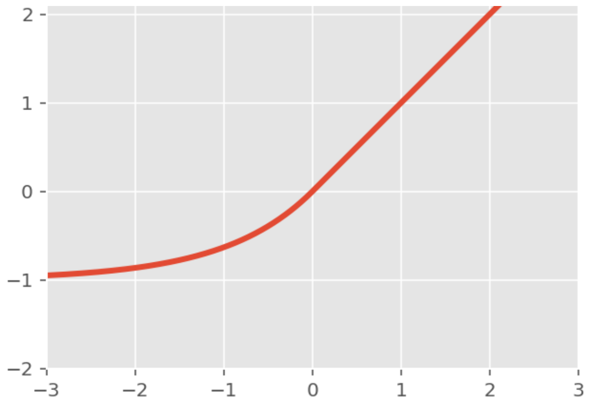
  - Avoids stuck-at-zero units
  - Weaker offset bias



- ELU

$$g(a) = \begin{cases} a, & a \geq 0 \\ e^{a} - 1, & a < 0 \end{cases}$$

  - No offset bias anymore
  - BUT: need to store activations



Recap: Glorot Initialization [Glorot & Bengio, '10]

- Variance of neuron activations
  - Suppose we have an input X with n components and a linear neuron with random weights W that spits out a number Y.
  - We *want the variance of the input and output of a unit to be the same*, therefore $n\,\mathrm{Var}(W_i)$ should be 1. This means

$$\mathrm{Var}(W_i) = \frac{1}{n} = \frac{1}{n_{\text{in}}}$$

  - Or for the backpropagated gradient

$$\mathrm{Var}(W_i) = \frac{1}{n_{\text{out}}}$$

  - As a compromise, Glorot & Bengio propose to use

$$\mathrm{Var}(W) = \frac{2}{n_{\text{in}} + n_{\text{out}}}$$

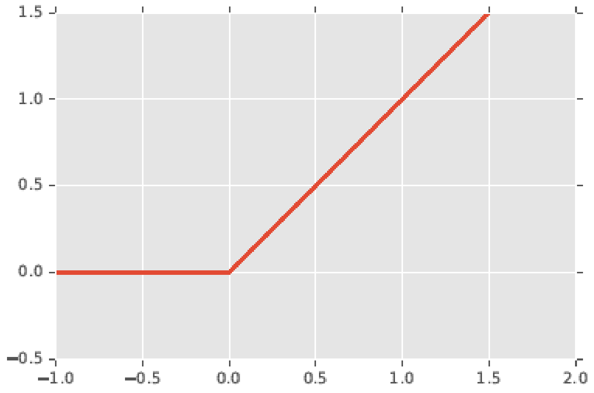
$\Rightarrow$ Randomly sample the weights with this variance. That's it.

Recap: He Initialization

[He et al., '15]

- Extension of Glorot Initialization to ReLU units
  - Use Rectified Linear Units (ReLU)

$$g(a) = \max\{0, a\}$$



  - Effect: gradient is propagated with a constant factor

$$\frac{\partial g(a)}{\partial a} = \begin{cases} 1, & a > 0 \\ 0, & \text{else} \end{cases}$$

- Same basic idea: Output should have the input variance
  - However, the Glorot derivation was based on tanh units, linearity assumption around zero does not hold for ReLU.
  - He et al. made the derivations, proposed to use instead

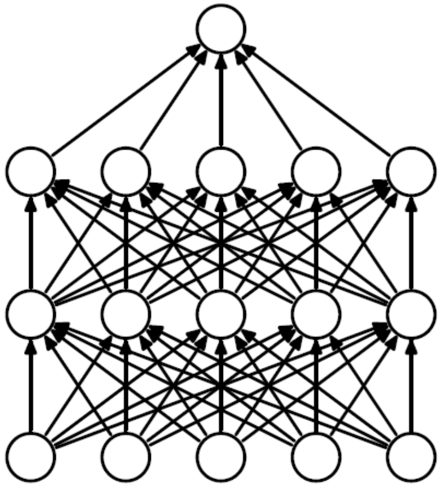
$$\mathrm{Var}(W) = \frac{2}{n_{\text{in}}}$$

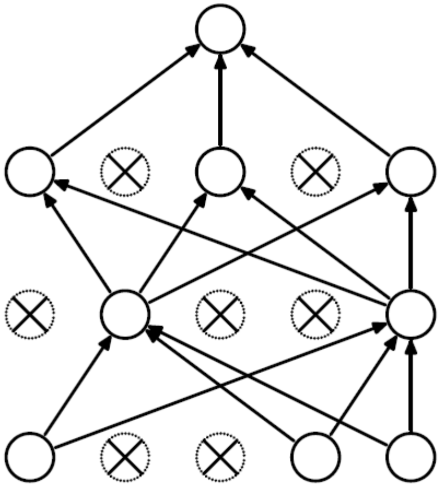
Recap: Batch Normalization [Ioffe & Szegedy ’14]

- Motivation
  - Optimization works best if all inputs of a layer are normalized.
- Idea
  - Introduce intermediate layer that centers the activations of the previous layer per minibatch.
  - I.e., perform transformations on all activations and undo those transformations when backpropagating gradients
- Effect
  - (Typically) much improved convergence

Recap: Dropout

[Srivastava, Hinton '12]


(a) Standard Neural Net

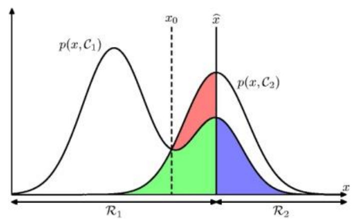

(b) After applying dropout.

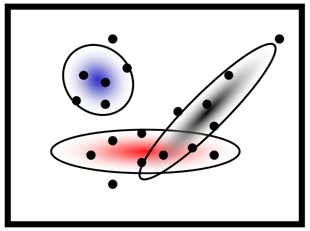
- Idea
  - Randomly switch off units during training.
  - Change network architecture for each data point, effectively training many different variants of the network.
  - When applying the trained network, multiply activations with the probability that the unit was set to zero.

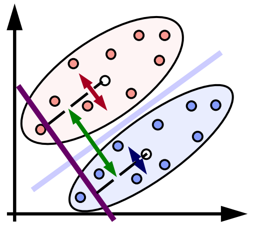
  $\Rightarrow$ Improved performance

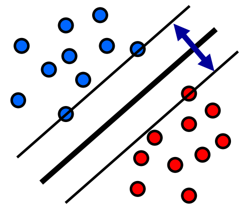
Course Outline

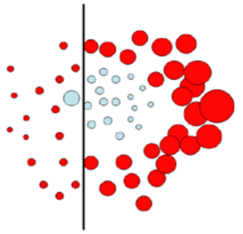
- Fundamentals
  - Bayes Decision Theory
  - Probability Density Estimation
- Classification Approaches
  - Linear Discriminants
  - Support Vector Machines
  - Ensemble Methods & Boosting
- Deep Learning
  - Foundations
  - Convolutional Neural Networks
  - Recurrent Neural Networks

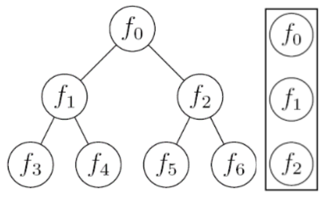


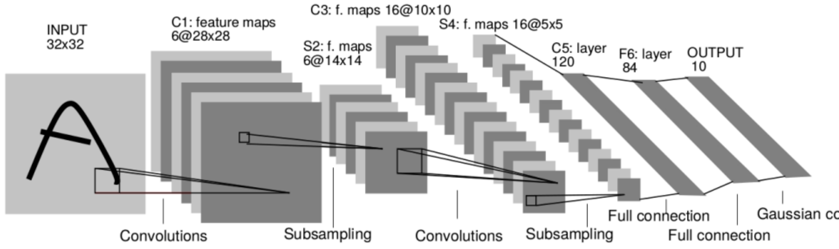




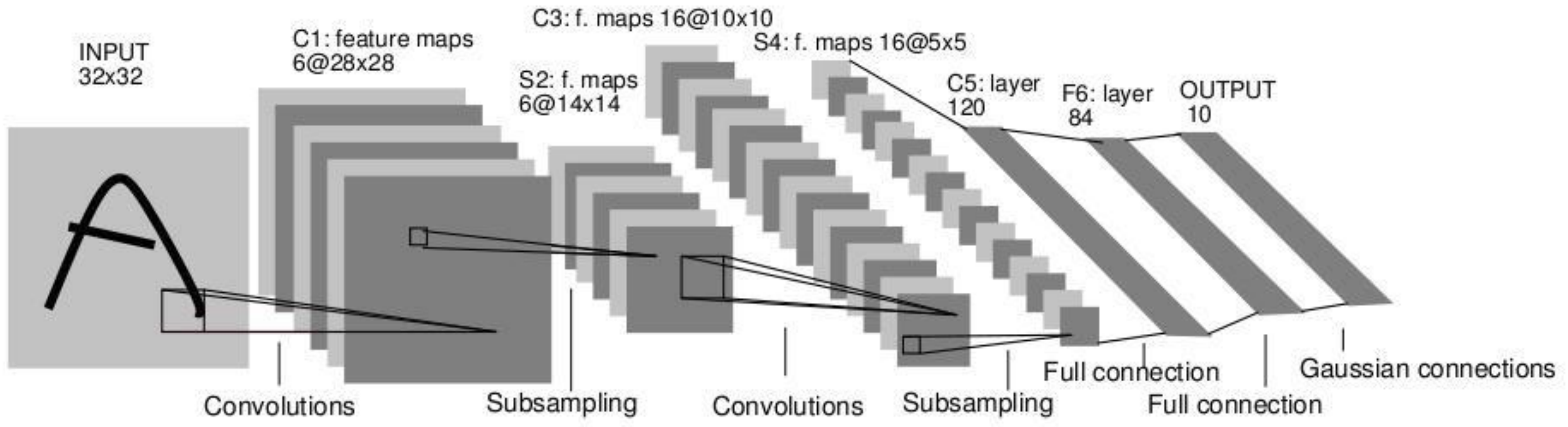








Recap: Convolutional Neural Networks



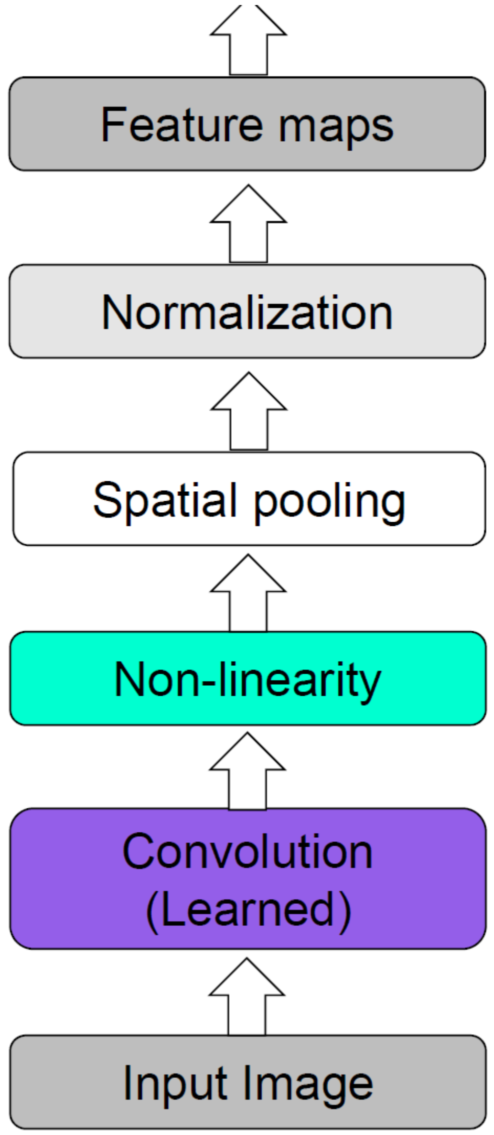
- Neural network with specialized connectivity structure
  - Stack multiple stages of feature extractors
  - Higher stages compute more global, more invariant features
  - Classification layer at the end

Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner, Gradient-based learning applied to document recognition, Proceedings of the IEEE 86(11): 2278–2324, 1998.

Slide credit: Svetlana Lazebnik

Recap: CNN Structure

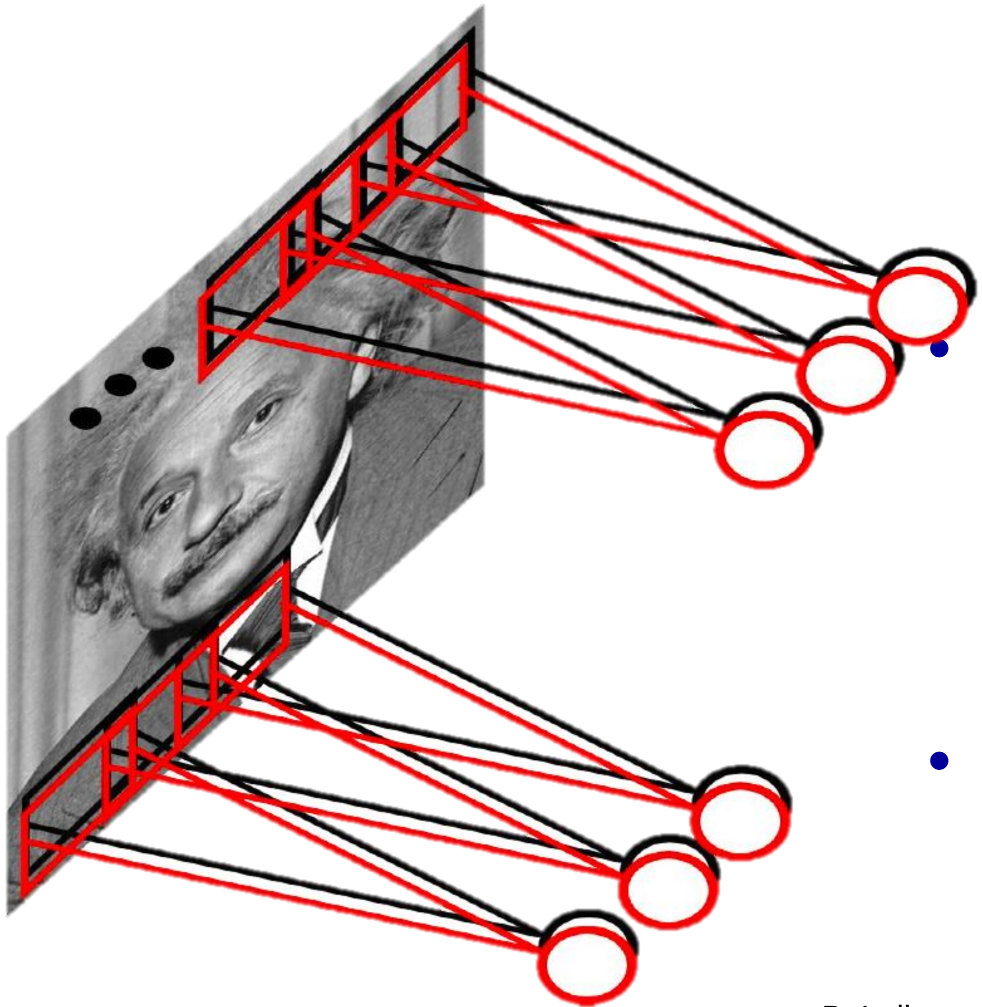
- Feed-forward feature extraction
  1. Convolve input with learned filters
  2. Non-linearity
  3. Spatial pooling
  4. (Normalization)
- Supervised training of convolutional filters by back-propagating classification error



Slide credit: Svetlana Lazebnik

Recap: Intuition of CNNs

see Exercise 5.1

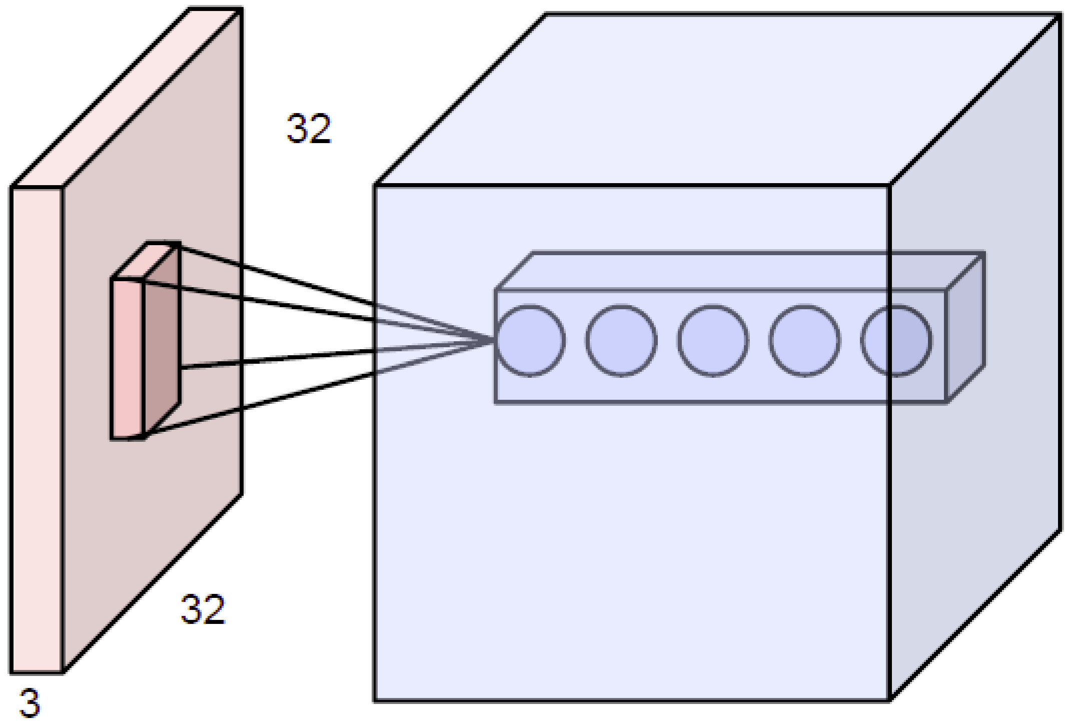


- Convolutional net
  - Share the same parameters across different locations
  - Convolutions with learned kernels
- Learn *multiple* filters
  - E.g. 1000×1000 image
    100 filters
    10×10 filter size

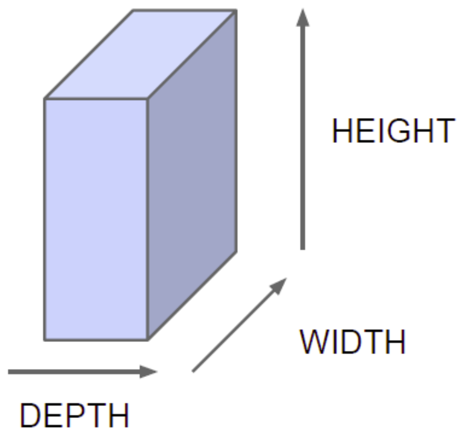
  $\Rightarrow$ only 10k parameters
- Result: Response map
  - size: $1000 \times 1000 \times 100$
  - Only memory, not params!

Image source: Yann LeCun

Recap: Convolution Layers



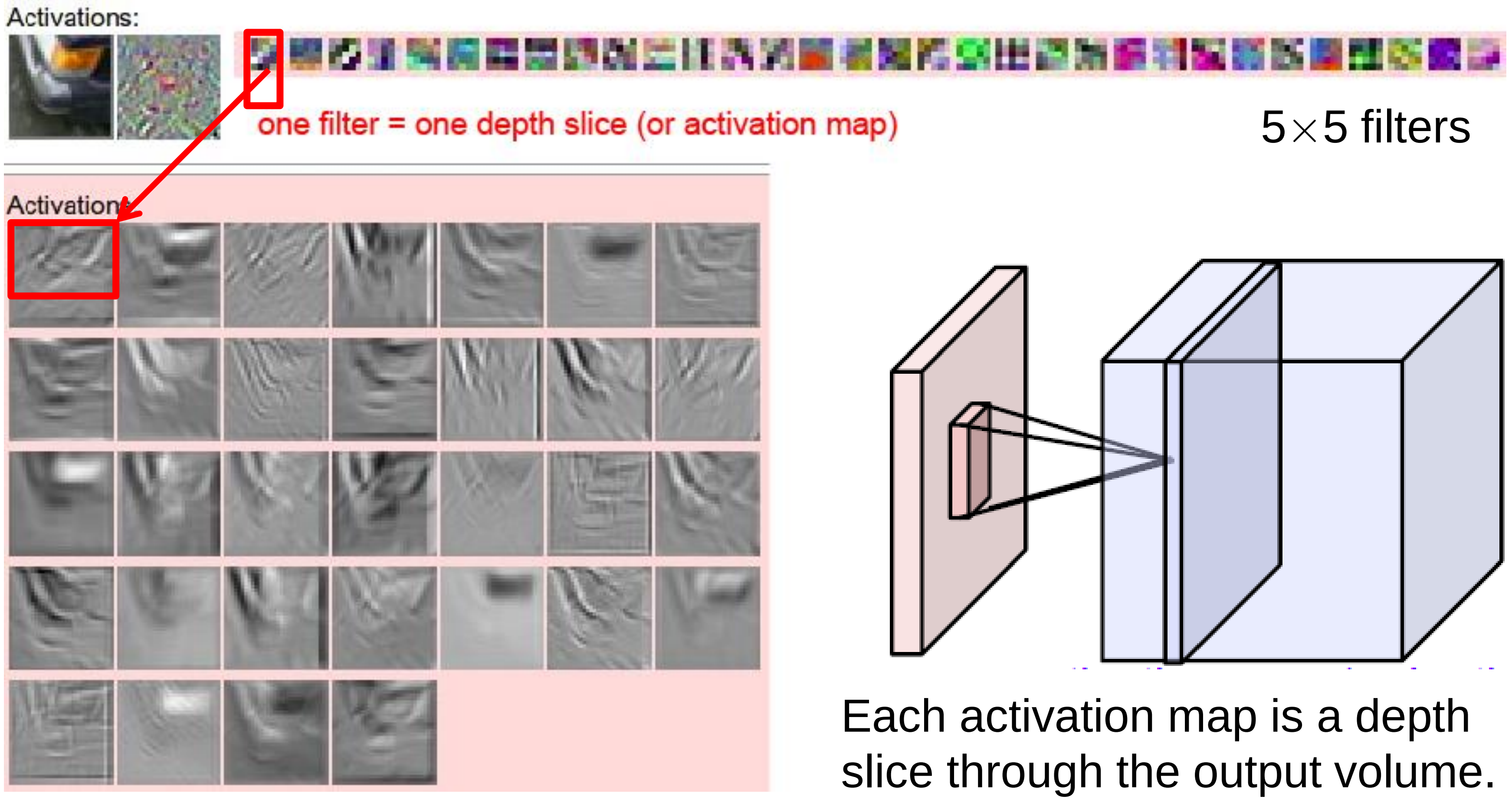
Naming convention:



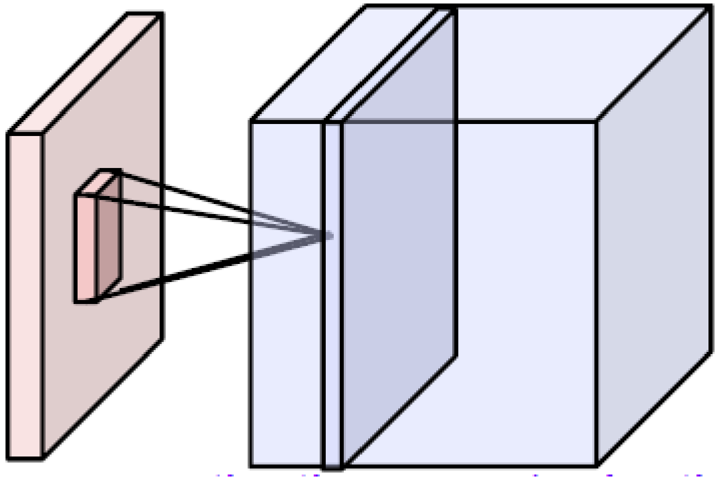
- All Neural Net activations arranged in 3 dimensions
  - Multiple neurons all looking at the same input region, stacked in depth
  - Form a single [1×1×depth] depth column in output volume.

Slide credit: FeiFei Li, Andrej Karpathy

Recap: Activation Maps



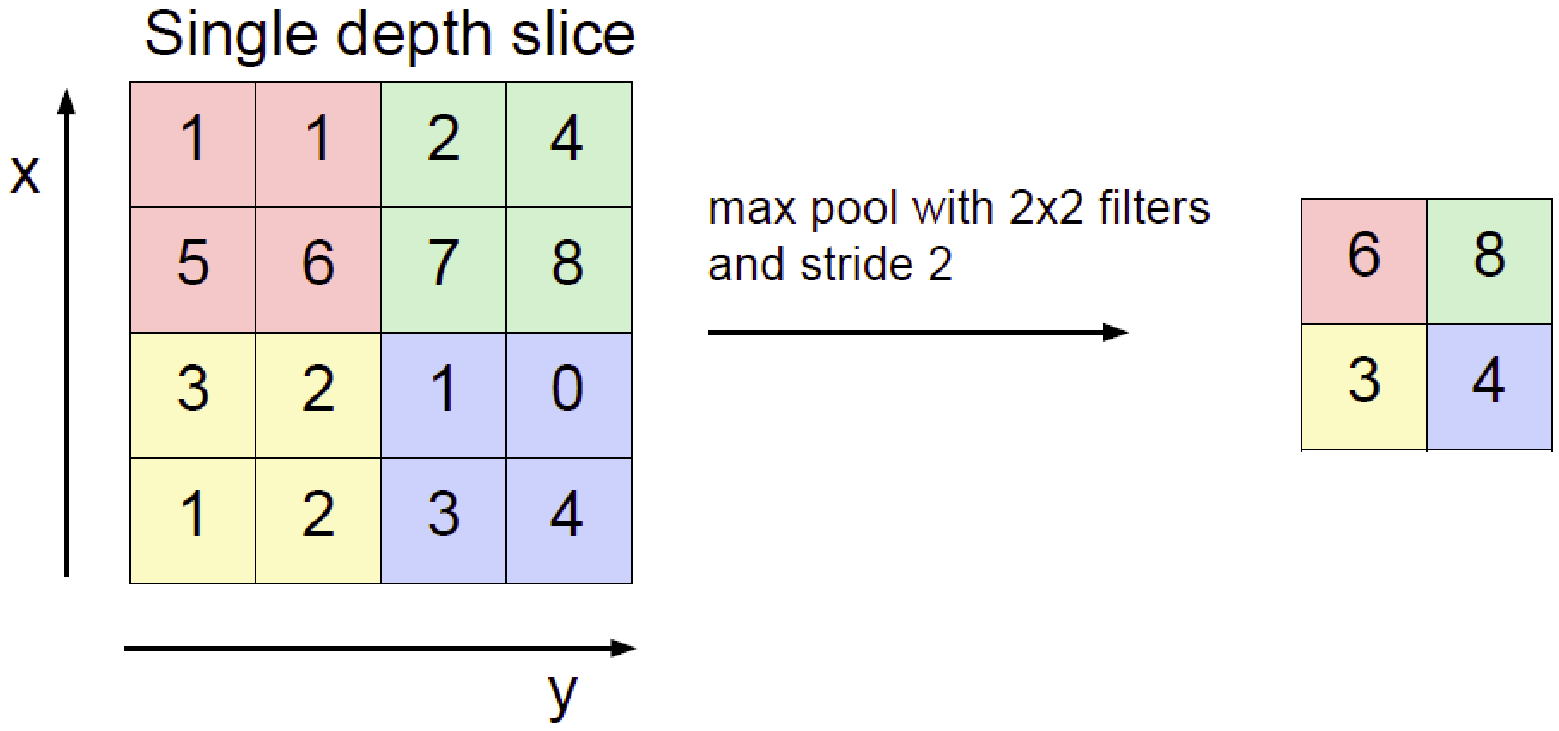
5×5 filters



Each activation map is a depth slice through the output volume.

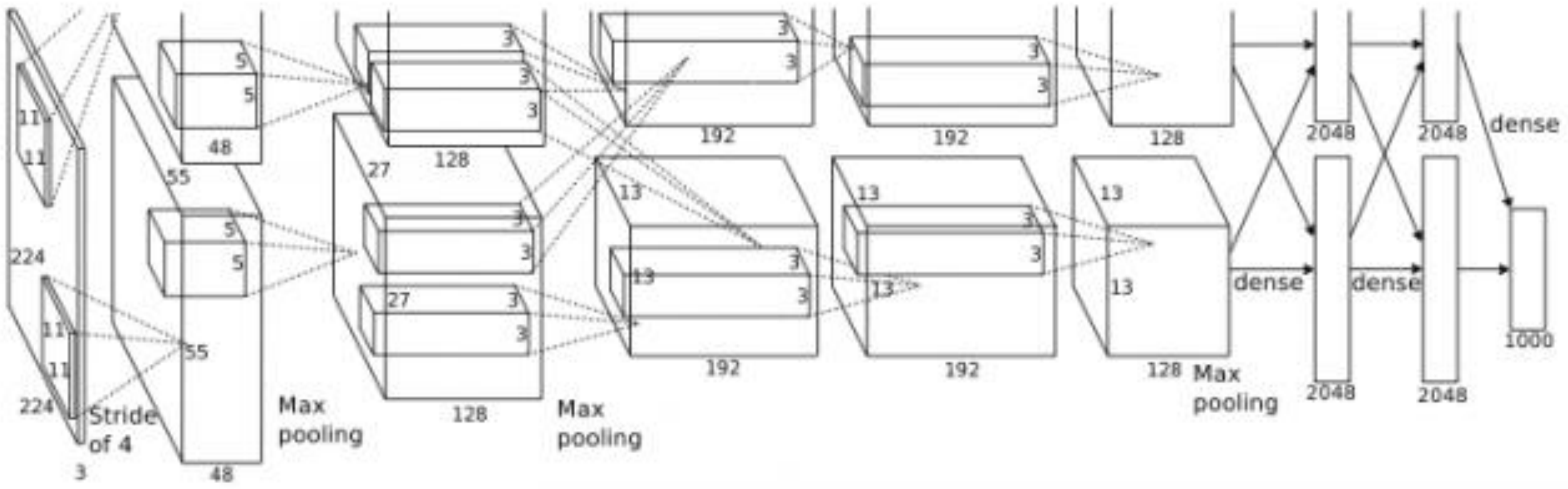
Activation maps

Recap: Pooling Layers



- Effect:
  - Make the representation smaller without losing too much information
  - Achieve robustness to translations

Recap: AlexNet (2012)



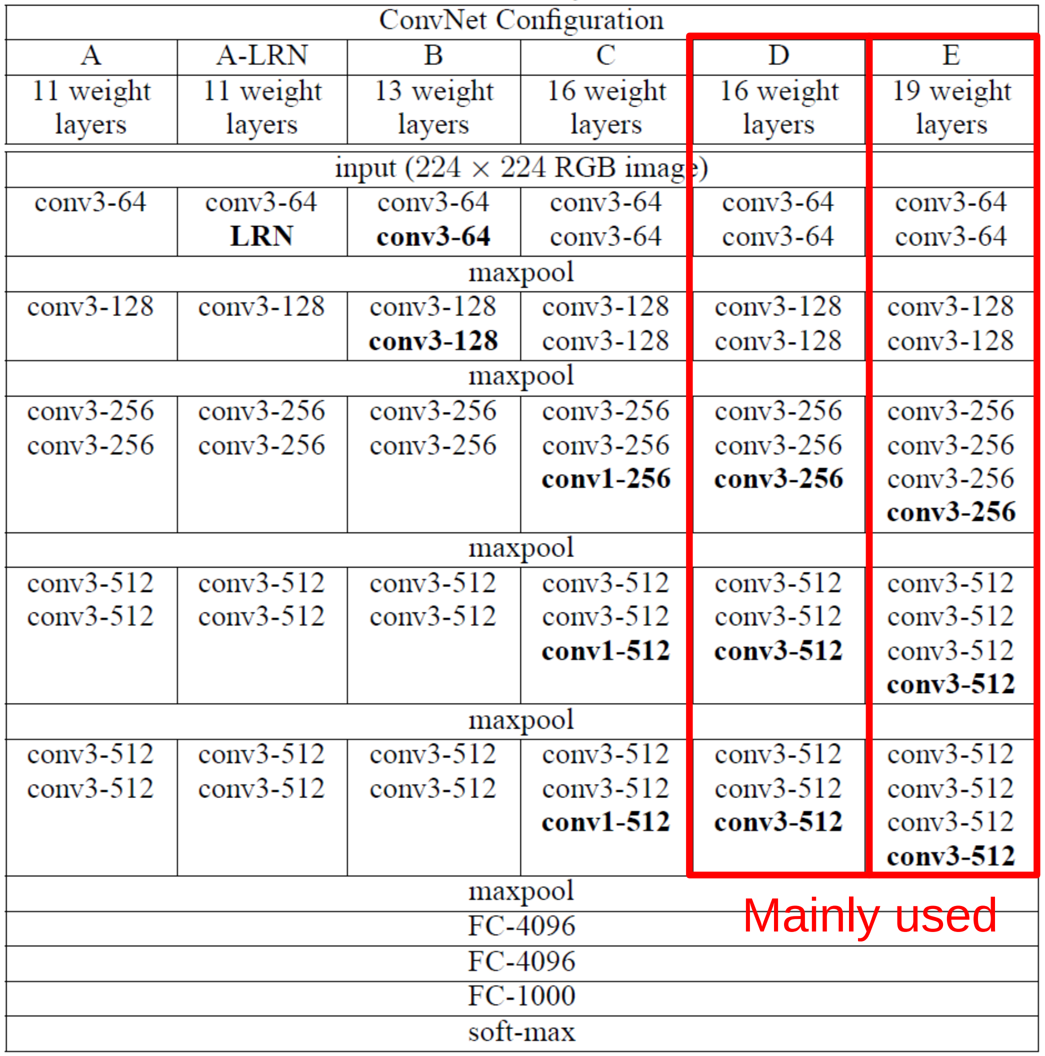
- Similar framework as LeNet, but
  - Bigger model (7 hidden layers, 650k units, 60M parameters)
  - More data (10^6 images instead of 10^3)
  - GPU implementation
  - Better regularization and up-to-date tricks for training (Dropout)

A. Krizhevsky, I. Sutskever, and G. Hinton, ImageNet Classification with Deep Convolutional Neural Networks, NIPS 2012.

Image source: A. Krizhevsky, I. Sutskever and G.E. Hinton, NIPS 2012

Recap: VGGNet (2014/15)

- Main ideas
  - Deeper network
  - Stacked convolutional layers with smaller filters (+ nonlinearity)
  - Detailed evaluation of all components
- Results
  - Improved ILSVRC top-5 error rate to 6.7%.



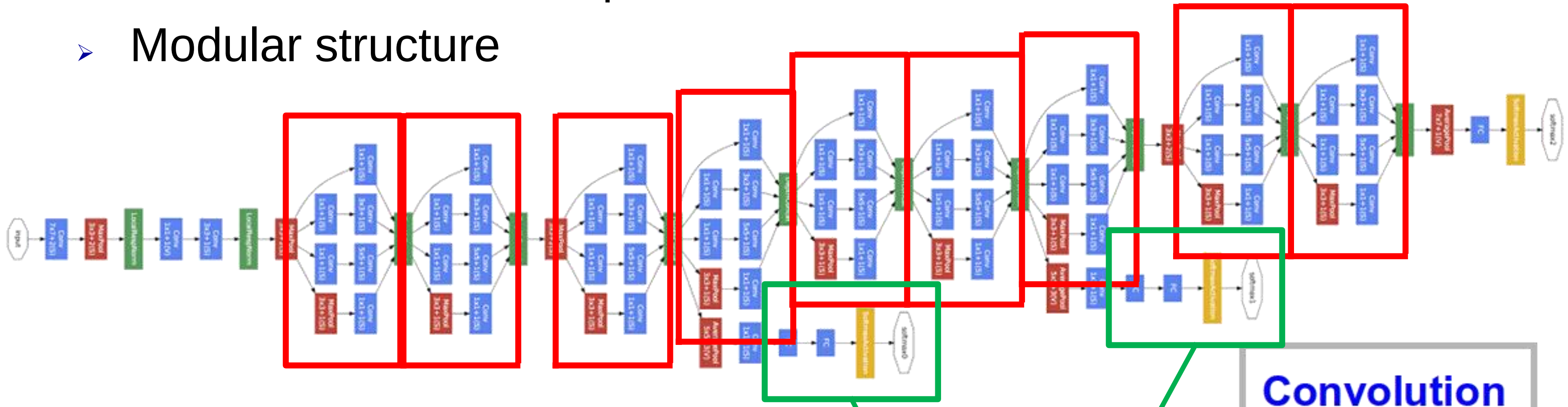
ConvNet Configuration					
A	A-LRN	B	C	D	E
11 weight layers	11 weight layers	13 weight layers	16 weight layers	16 weight layers	19 weight layers
input (224 × 224 RGB image)					
conv3-64	conv3-64 **LRN**	conv3-64 **conv3-64**	conv3-64 conv3-64	conv3-64 conv3-64	conv3-64 conv3-64
maxpool					
conv3-128	conv3-128	conv3-128 **conv3-128**	conv3-128 conv3-128	conv3-128 conv3-128	conv3-128 conv3-128
maxpool					
conv3-256 conv3-256	conv3-256 conv3-256	conv3-256 conv3-256	conv3-256 conv3-256 **conv1-256**	conv3-256 conv3-256 **conv3-256**	conv3-256 conv3-256 conv3-256 **conv3-256**
maxpool					
conv3-512 conv3-512	conv3-512 conv3-512	conv3-512 conv3-512	conv3-512 conv3-512 **conv1-512**	conv3-512 conv3-512 **conv3-512**	conv3-512 conv3-512 conv3-512 **conv3-512**
maxpool					
conv3-512 conv3-512	conv3-512 conv3-512	conv3-512 conv3-512	conv3-512 conv3-512 **conv1-512**	conv3-512 conv3-512 **conv3-512**	conv3-512 conv3-512 conv3-512 **conv3-512**
maxpool					
FC-4096					
FC-4096					
FC-1000					
soft-max					

Mainly used

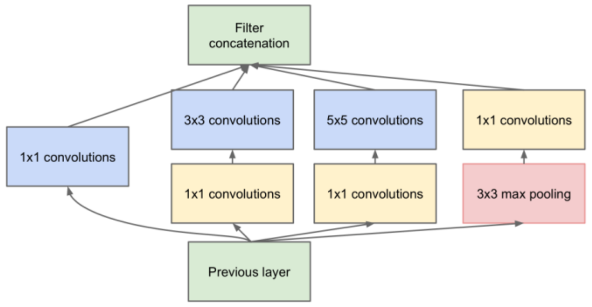
Image source: Simonyan & Zisserman

Recap: GoogLeNet (2014)

- Ideas:
  - Learn features at multiple scales
  - Modular structure



Inception module
+ copies
Auxiliary classification outputs for training the lower layers (deprecated)
Convolution
Pooling
Softmax
Other



(b) Inception module with dimension reductions

Image source: Szegedy et al.

Discussion

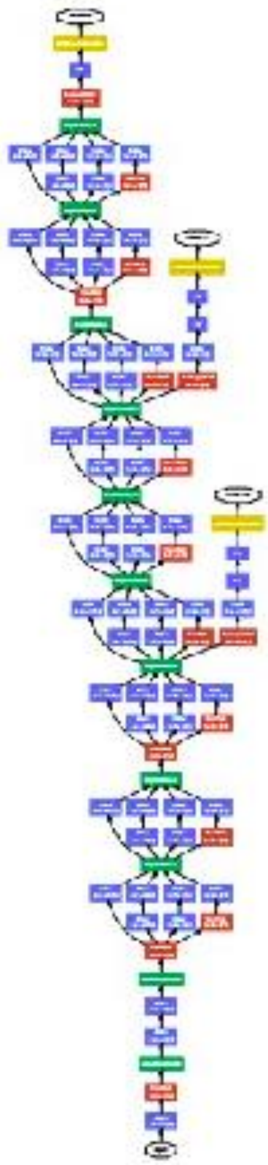
- GoogLeNet
  - 12× fewer parameters than AlexNet

  ⇒ ~5M parameters
  - *Where does the main reduction come from?*

  ⇒ From throwing away the fully connected (FC) layers.
- Effect
  - After last pooling layer, volume is of size [7×7×1024]
  - Normally you would place the first 4096-D FC layer here (Many million params).
  - Instead: use Average pooling in each depth slice:

  ⇒ Reduces the output to [1×1×1024].

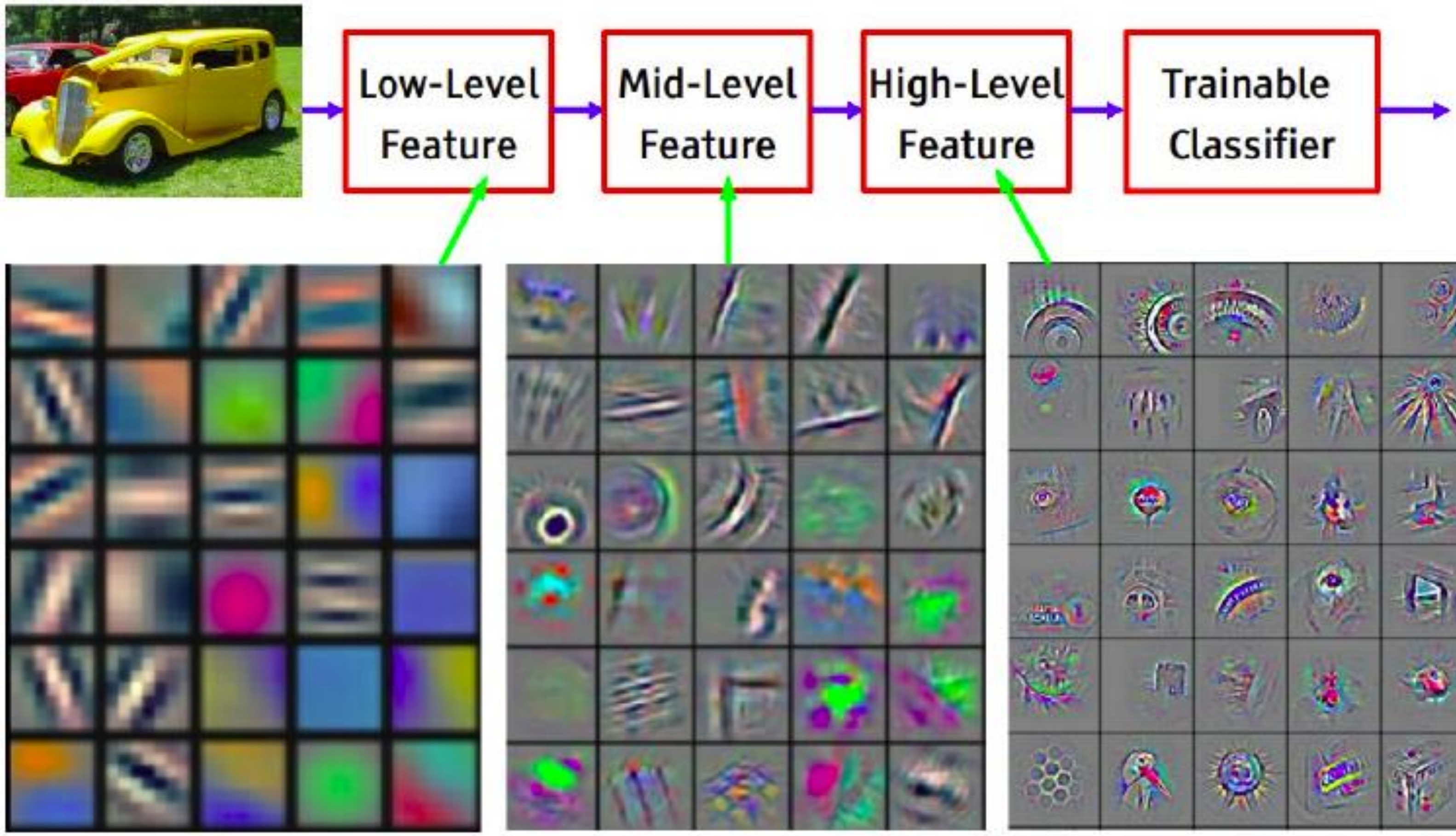
  ⇒ Performance actually improves by 0.6% compared to when using FC layers (less overfitting?)



Slide credit: Andrej Karpathy

Image source: Szegedy et al.

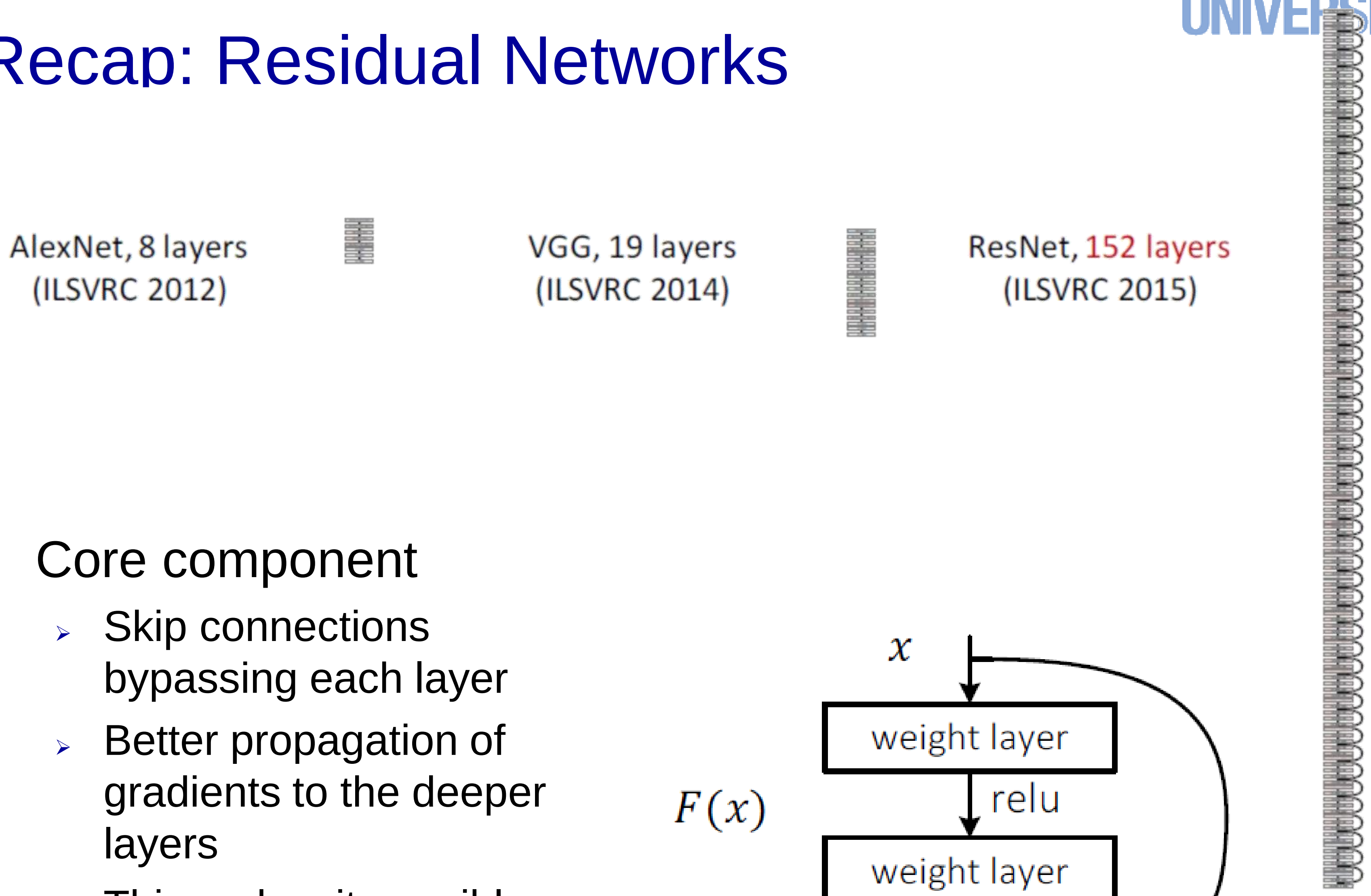
Recap: Visualizing CNNs



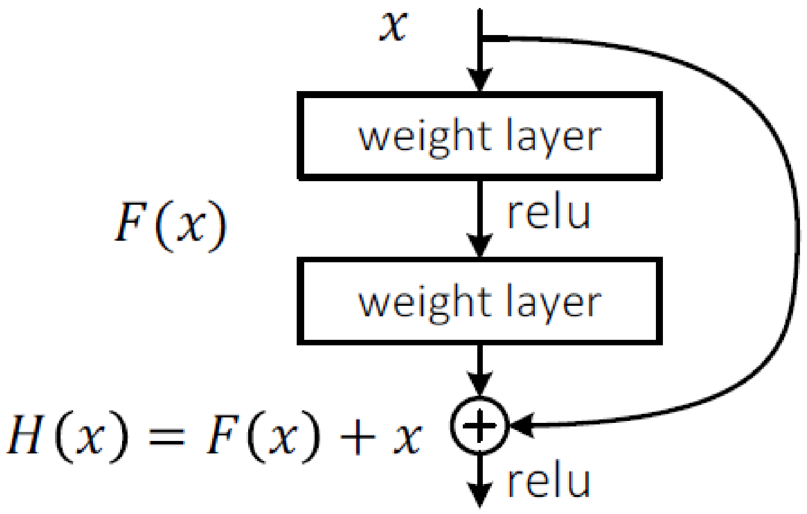
Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

Slide credit: Yann LeCun

Recap: Residual Networks

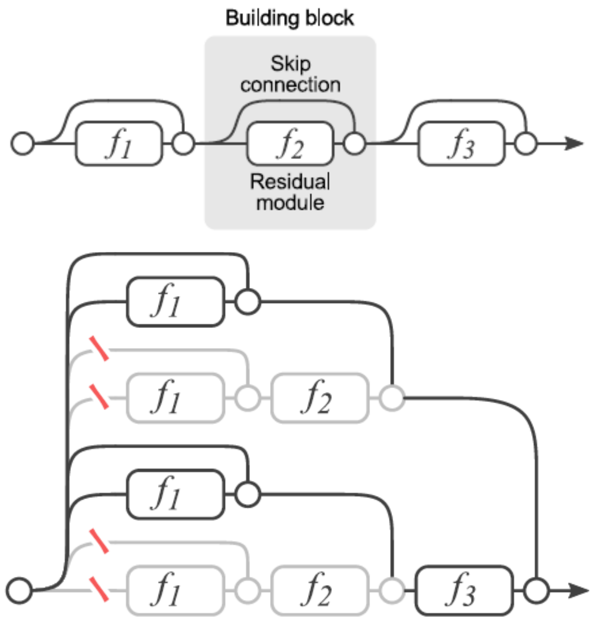


- Core component
  - Skip connections bypassing each layer
  - Better propagation of gradients to the deeper layers
  - This makes it possible to train (much) deeper networks.



Recap: Analysis of ResNets

- The effective paths in ResNets are relatively shallow
  - Effectively only 5-17 active modules
- This explains the resilience to deletion
  - Deleting any single layer only affects a subset of paths (and the shorter ones less than the longer ones).
- New interpretation of ResNets
  - ResNets work by creating an ensemble of relatively shallow paths
  - Making ResNets deeper increases the size of this ensemble
  - Excluding longer paths from training does not negatively affect the results.



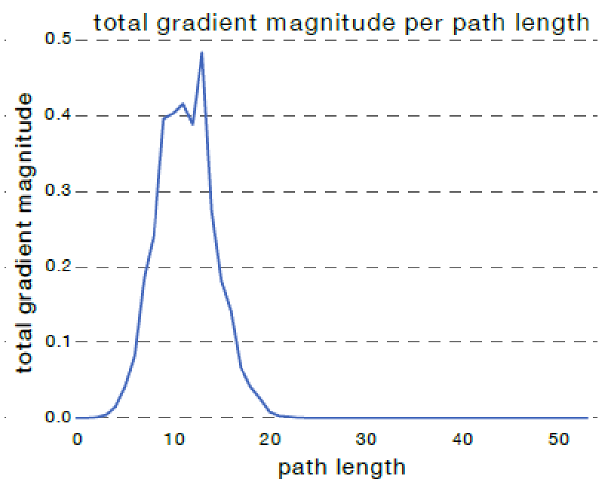
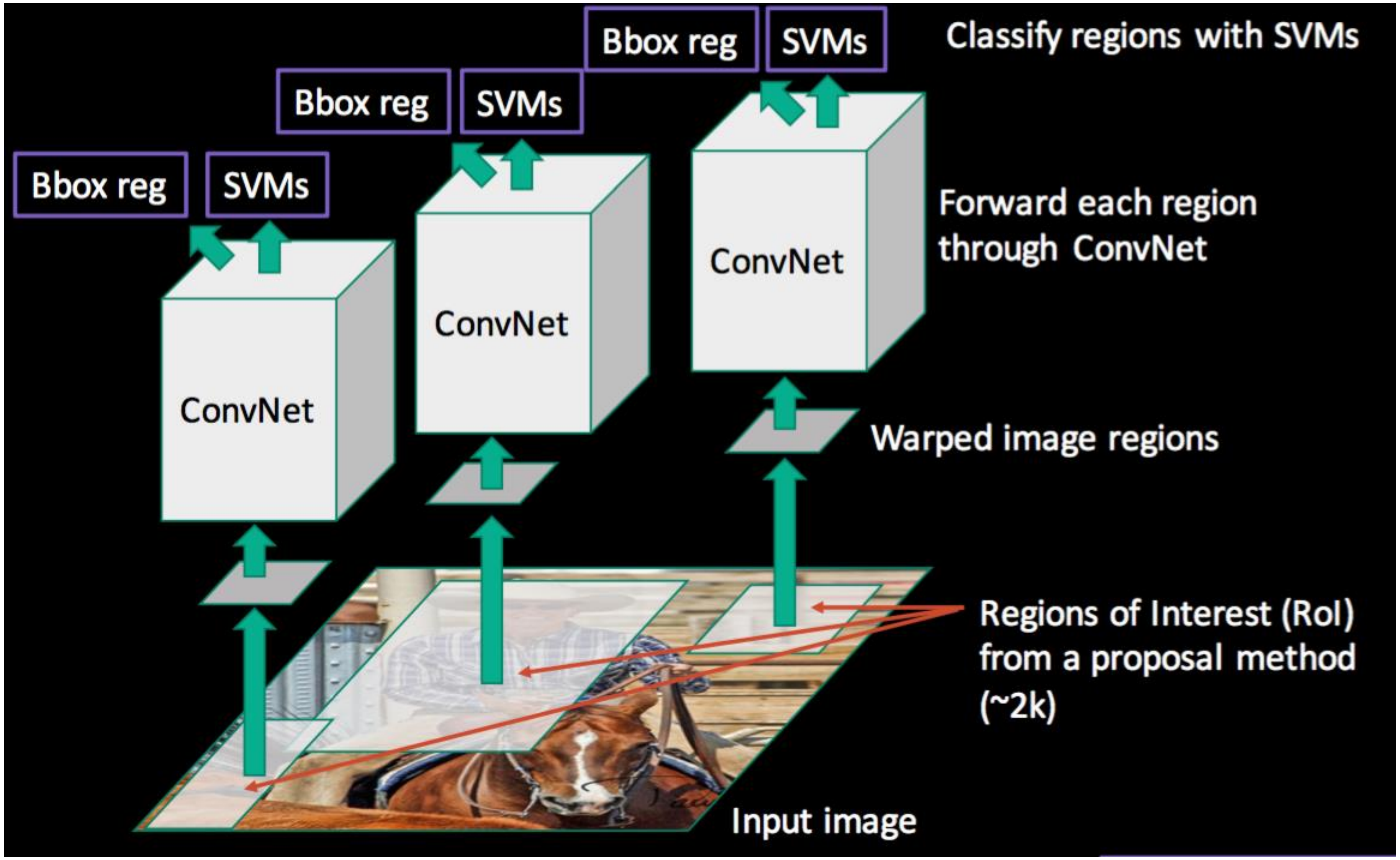


Image source: Veit et al., 2016

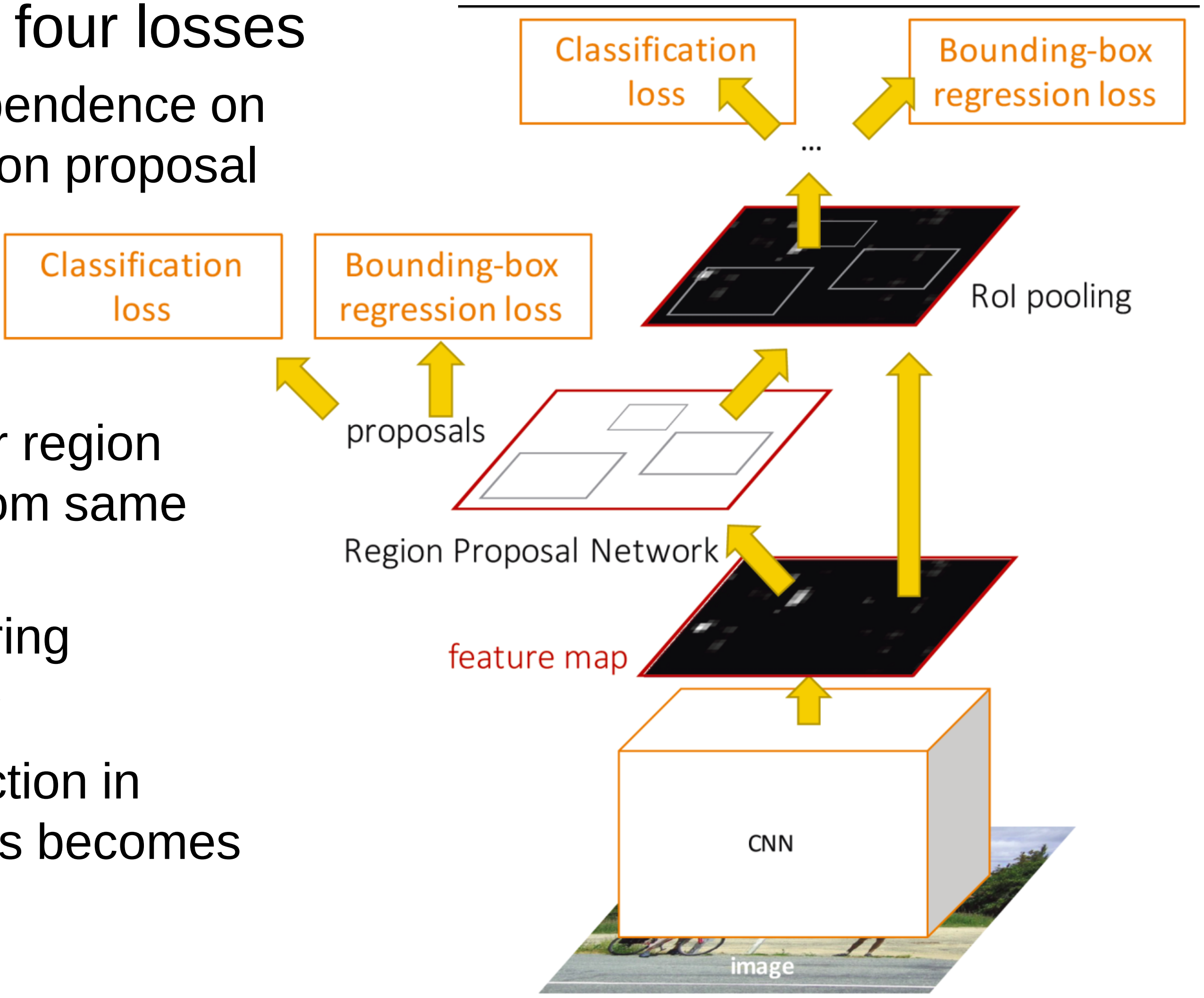
Recap: R-CNN for Object Detection


Bbox reg
SVMs
Classify regions with SVMs
ConvNet
Forward each region through ConvNet
Warped image regions
Regions of Interest (RoI) from a proposal method (~2k)
Input image

Slide credit: Ross Girshick

Recap: Faster R-CNN for Object Detection

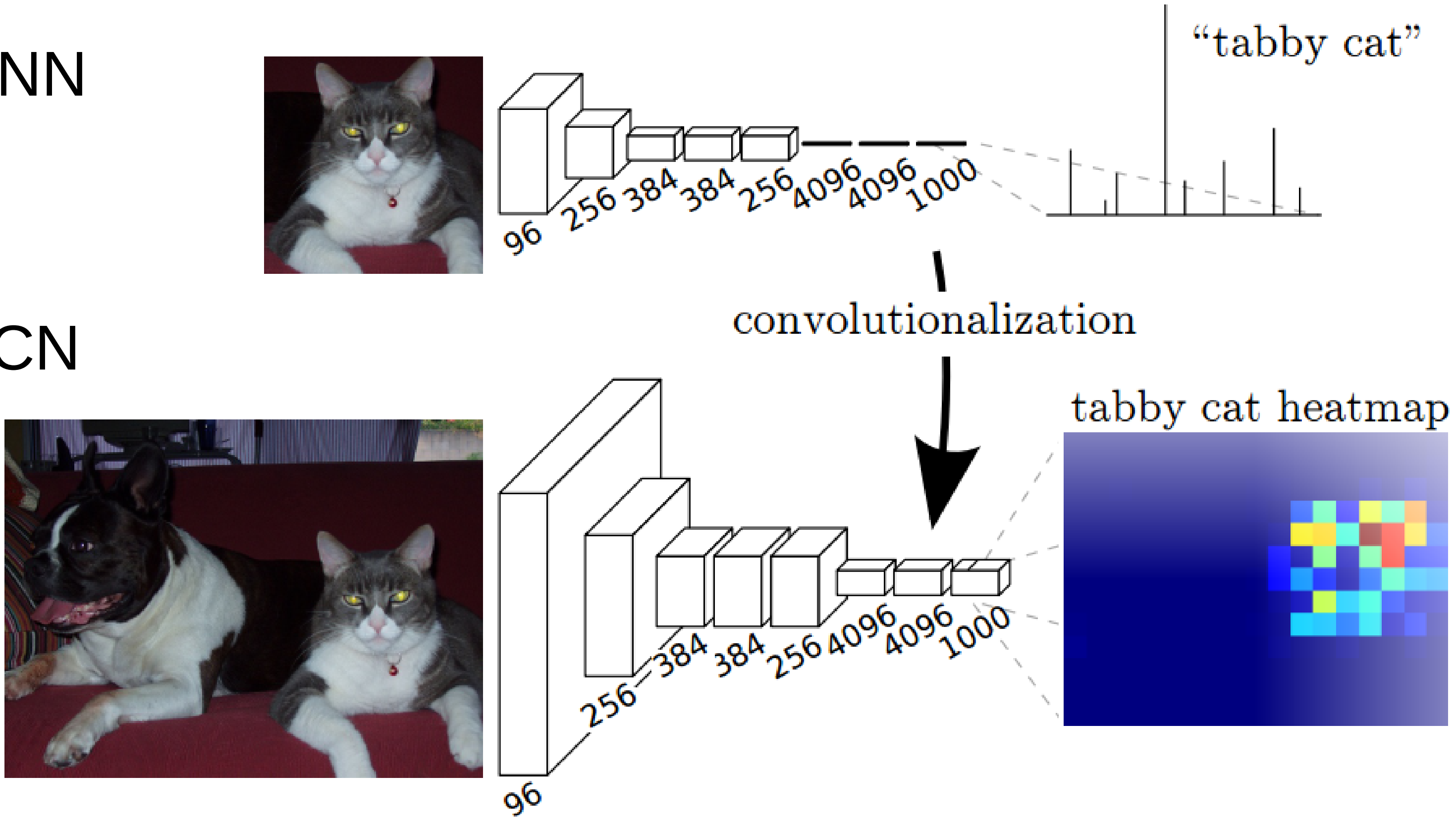
- One network, four losses
  - Remove dependence on external region proposal algorithm.
  - Instead, infer region proposals from same CNN.
  - Feature sharing
  - Joint training
  - ⇒ Object detection in a single pass becomes possible.



Slide credit: Ross Girshick

Recap: Fully Convolutional Networks

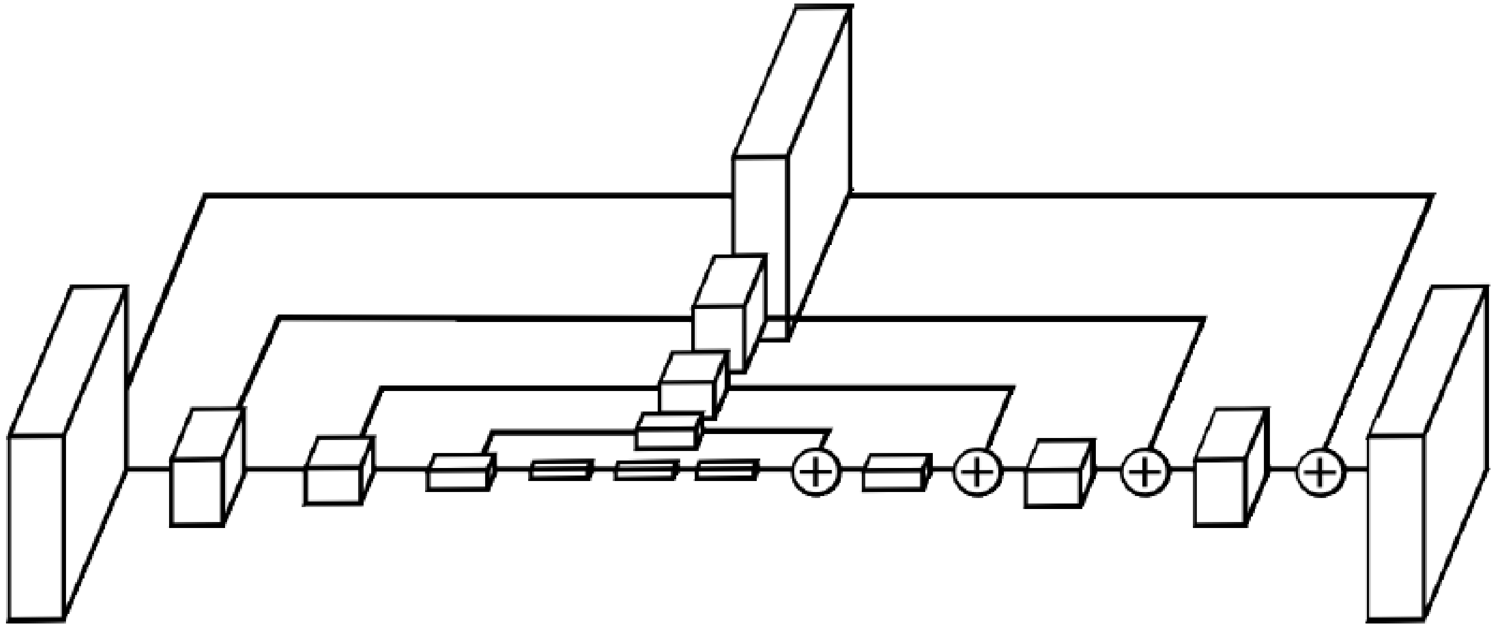
- CNN
- FCN



- Intuition
  - Think of FCNs as performing a sliding-window classification, producing a heatmap of output scores for each class

Image source: Long, Shelhamer, Darrell

Recap: Semantic Image Segmentation



- Encoder-Decoder Architecture
  - Problem: FCN output has low resolution
  - Solution: perform upsampling to get back to desired resolution
  - Use skip connections to preserve higher-resolution information

Image source: Newell et al.

Course Outline

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  - Probability Density Estimation
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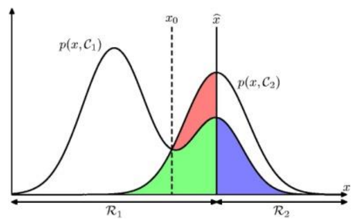
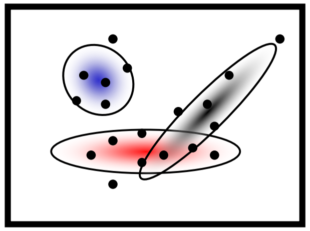
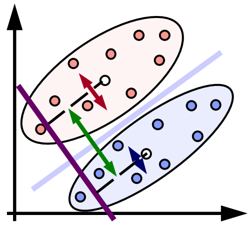
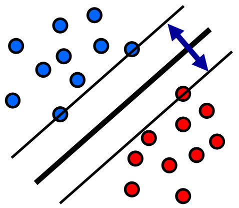
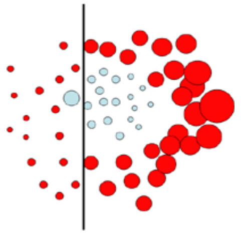
  - Linear Discriminants
  - Support Vector Machines
  - Ensemble Methods & Boosting
- Deep Learning
  - Foundations
  - Convolutional Neural Networks
  - Recurrent Neural Networks

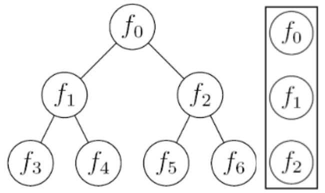


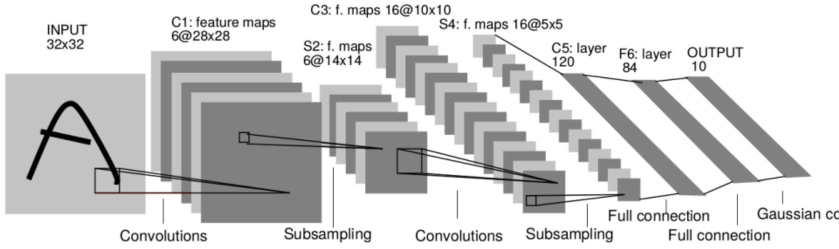




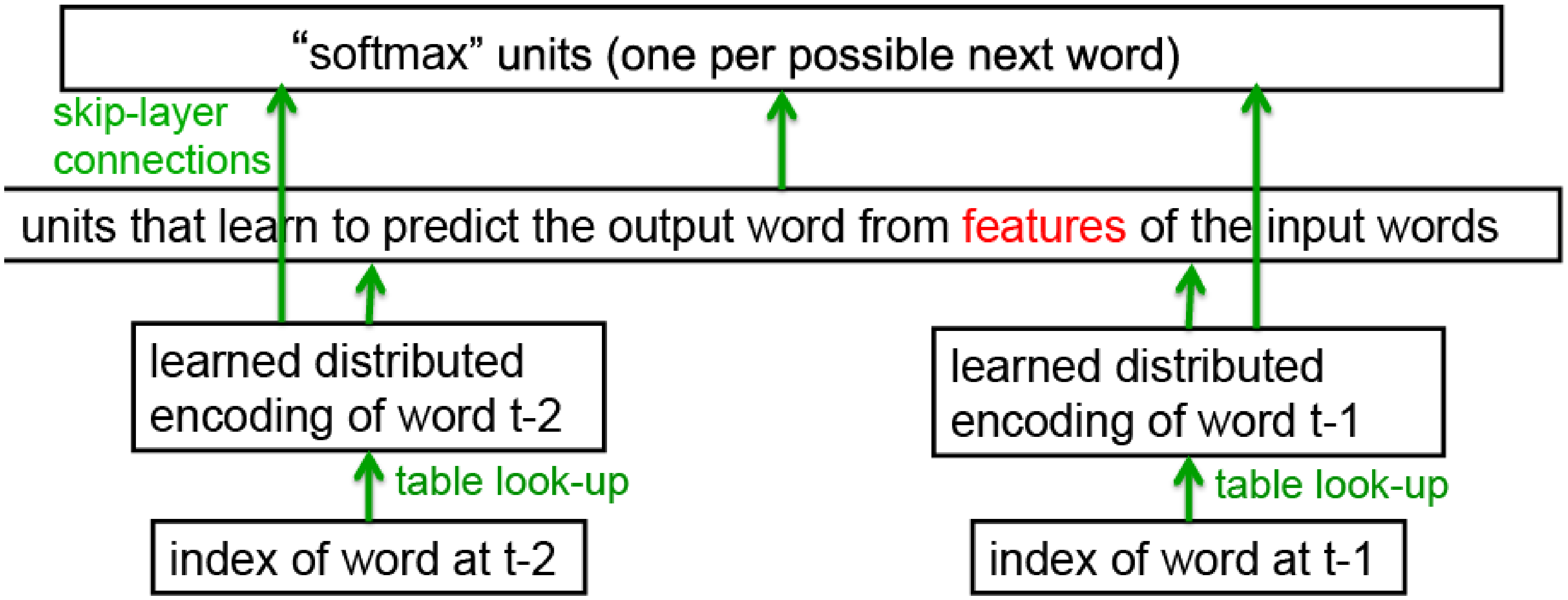








Recap: Neural Probabilistic Language Model


"softmax" units (one per possible next word)
skip-layer connections
units that learn to predict the output word from features of the input words
learned distributed encoding of word t-2
learned distributed encoding of word t-1
table look-up
table look-up
index of word at t-2
index of word at t-1

- Core idea
  - Learn a shared distributed encoding (word embedding) for the words in the vocabulary.

Y. Bengio, R. Ducharme, P. Vincent, C. Jauvin, A Neural Probabilistic Language Model, In JMLR, Vol. 3, pp. 1137-1155, 2003.

Image source: Geoff Hinton

Recap: word2vec

- Goal
  - Make it possible to learn high-quality word embeddings from huge data sets (billions of words in training set).
- Approach
  - Define two alternative learning tasks for learning the embedding:
    - "Continuous Bag of Words" (CBOW)
    - "Skip-gram"
  - Designed to require fewer parameters.

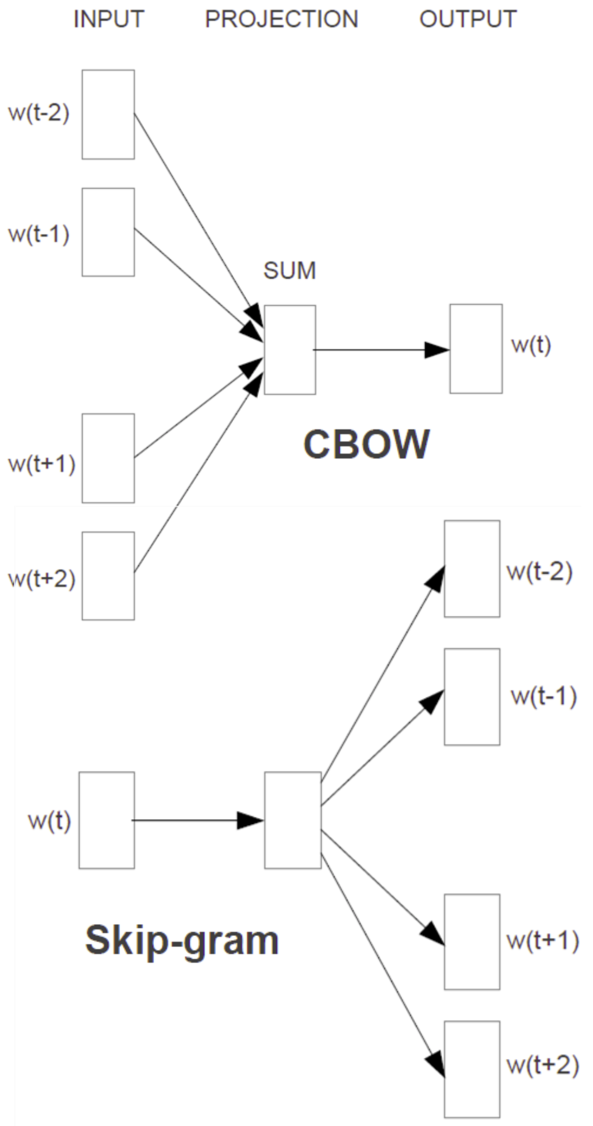


Image source: Mikolov et al., 2015

Recap: word2vec CBOW Model

- Continuous BOW Model
  - Remove the non-linearity from the hidden layer
  - Share the projection layer for all words (their vectors are averaged)

$\Rightarrow$ Bag-of-Words model (order of the words does not matter anymore)

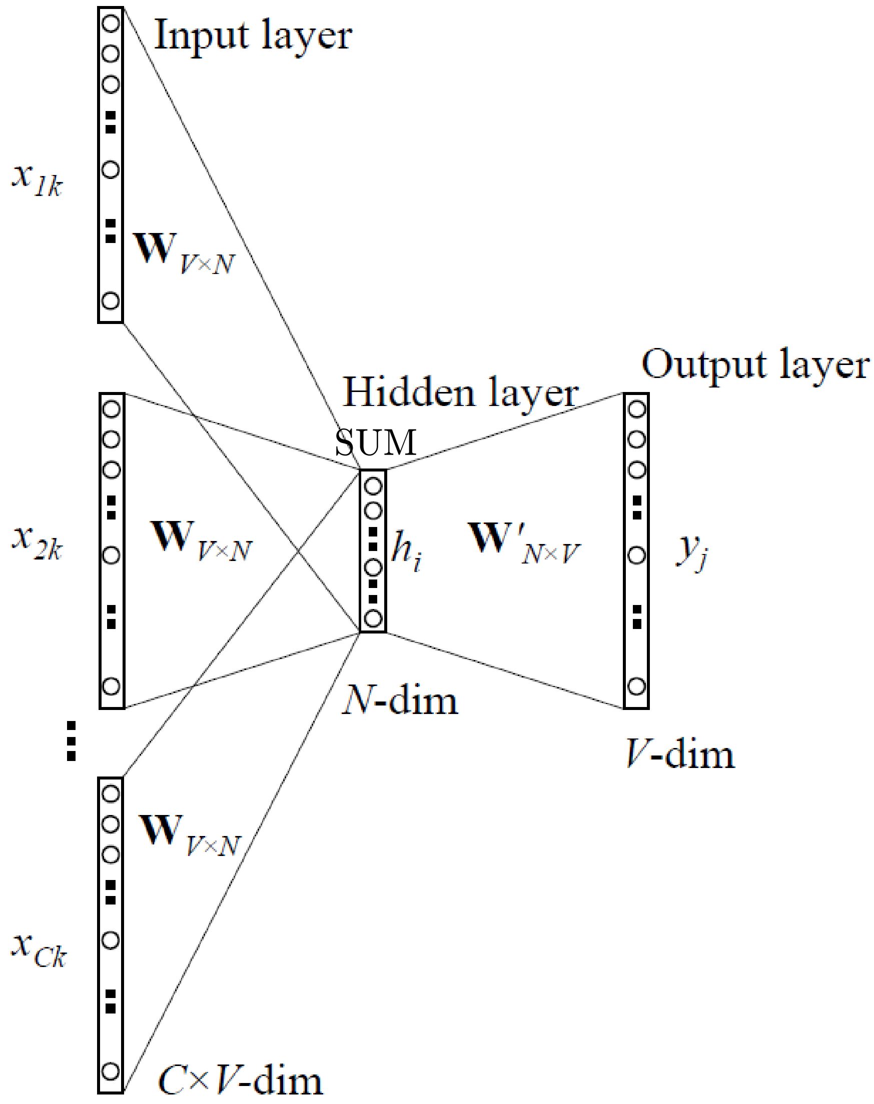


Image source: Xin Rong, 2015

Recap: word2vec Skip-Gram Model

- Continuous Skip-Gram Model
  - Similar structure to CBOW
  - Instead of predicting the current word, predict words within a certain range of the current word.
  - Give less weight to the more distant words

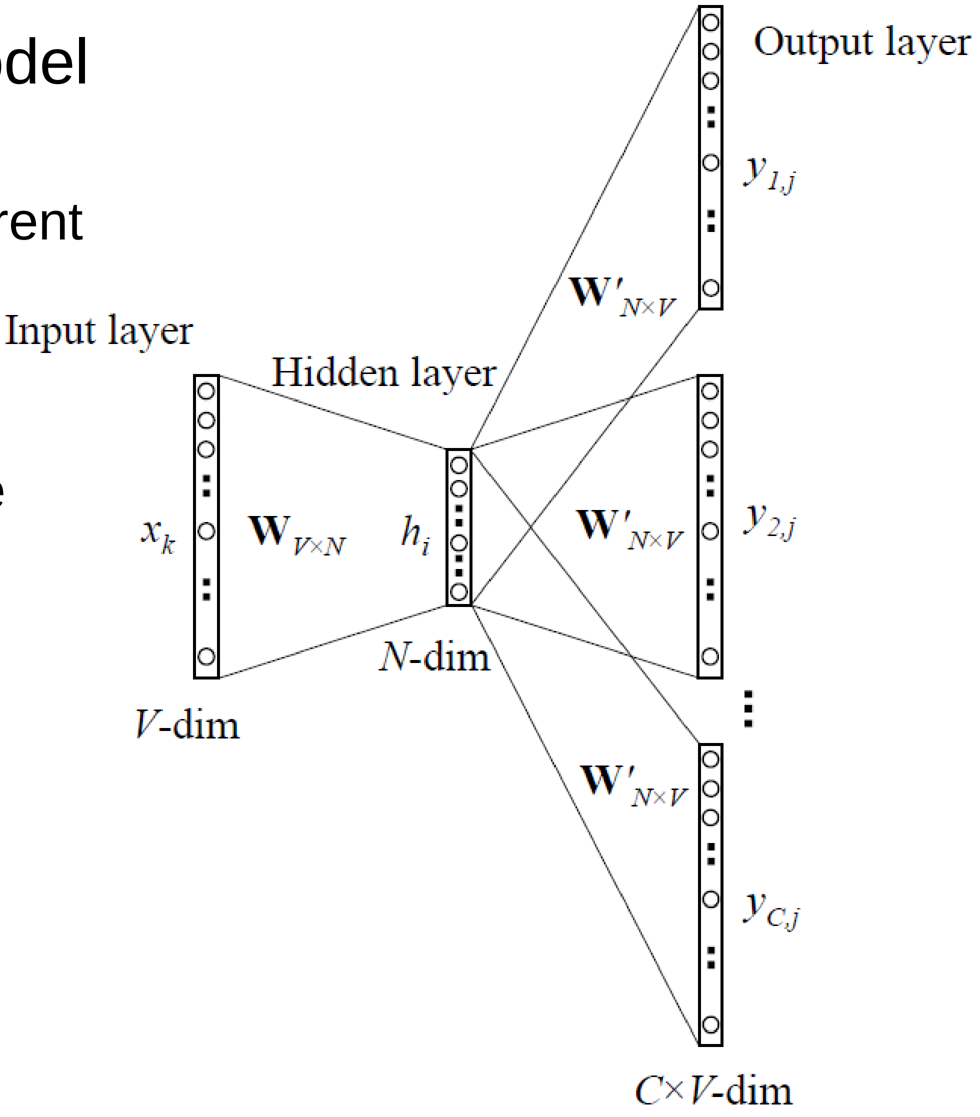


Image source: Xin Rong, 2015

Recap: Problems with 100k-1M outputs

- Weight matrix gets huge!
  - Example: CBOW model
  - One-hot encoding for inputs

  $\Rightarrow$ Input-hidden connections are just vector lookups.

  - This is not the case for the hidden-output connections!
  - State h is not one-hot, and vocabulary size is 1M.

  $\Rightarrow$ $\mathbf{W}'_{N\times V}$ has 300×1M entries

- Softmax gets expensive!
  - Need to compute normalization over 100k-1M outputs

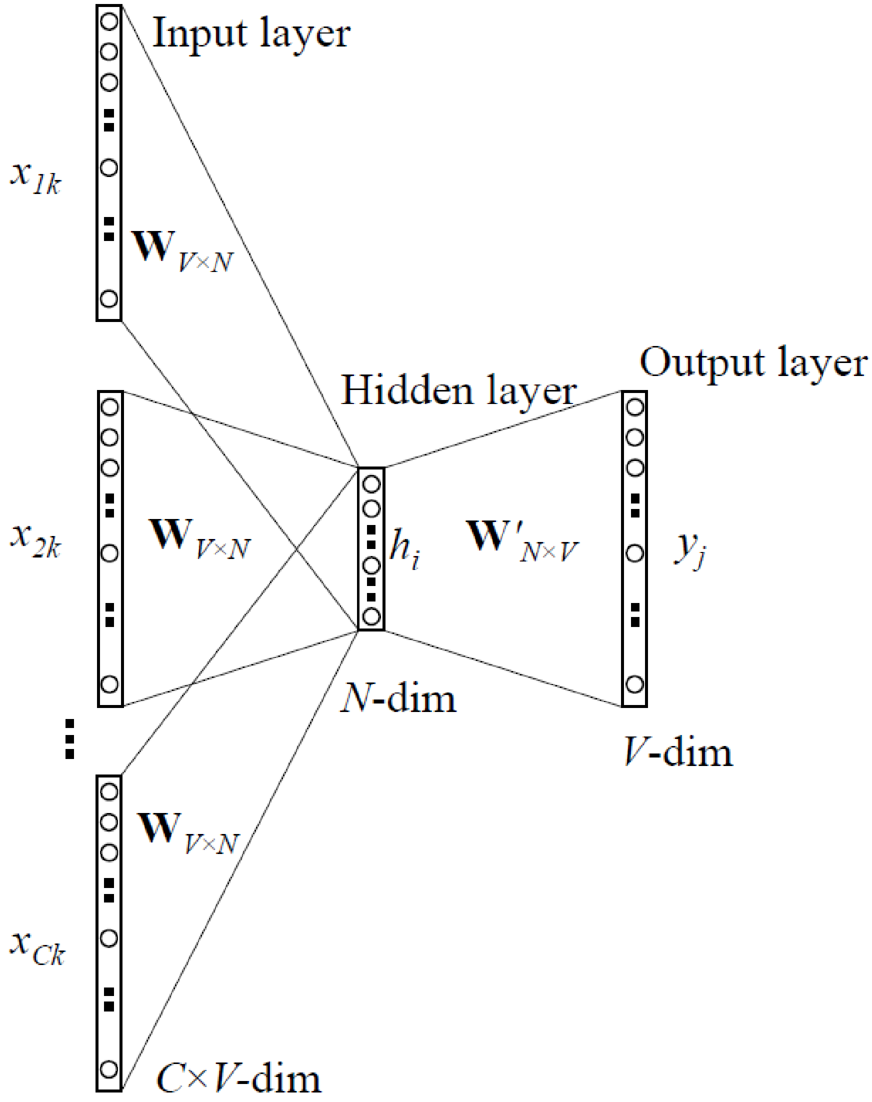
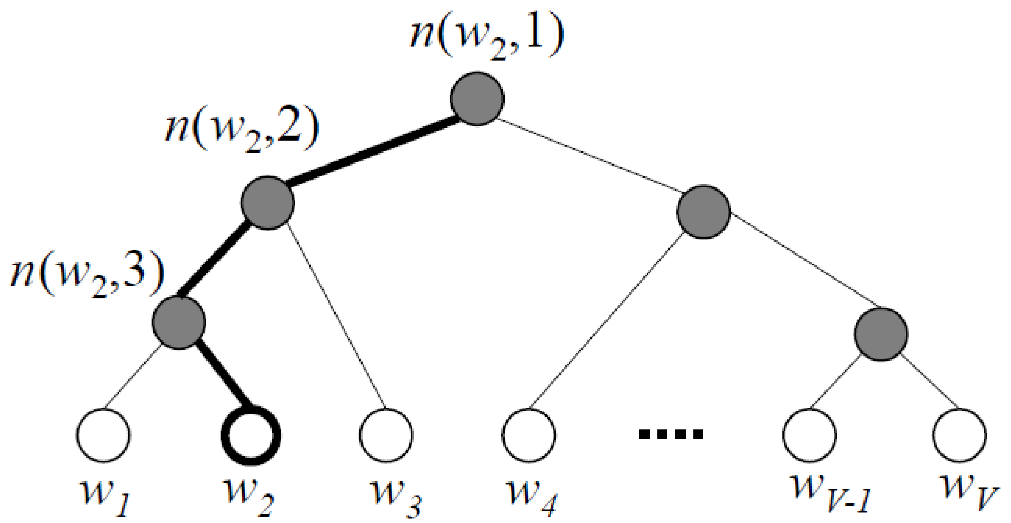


Image source: Xin Rong, 2015

Recap: Hierarchical Softmax

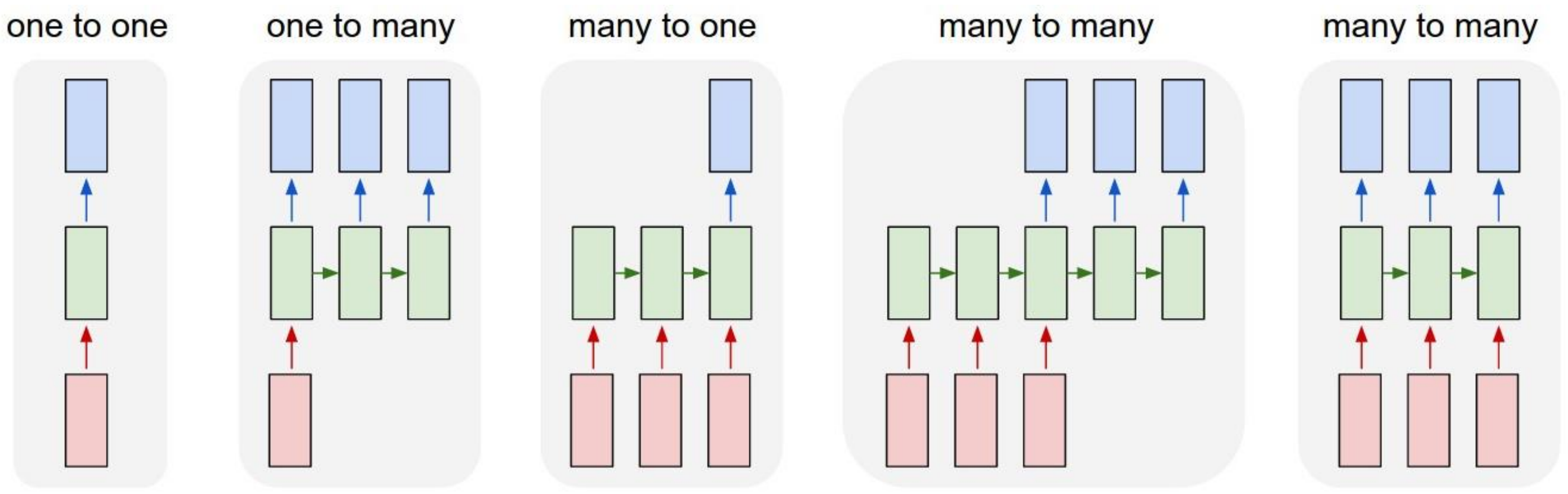


- Idea
  - Organize words in binary search tree, words are at leaves
  - Factorize probability of word w_0 as a product of node probabilities along the path.
  - Learn a linear decision function $y = v_{n(w,j)} \cdot h$ at each node to decide whether to proceed with left or right child node.

$\Rightarrow$ Decision based on output vector of hidden units directly.

Image source: Xin Rong, 2015

Recap: Recurrent Neural Networks

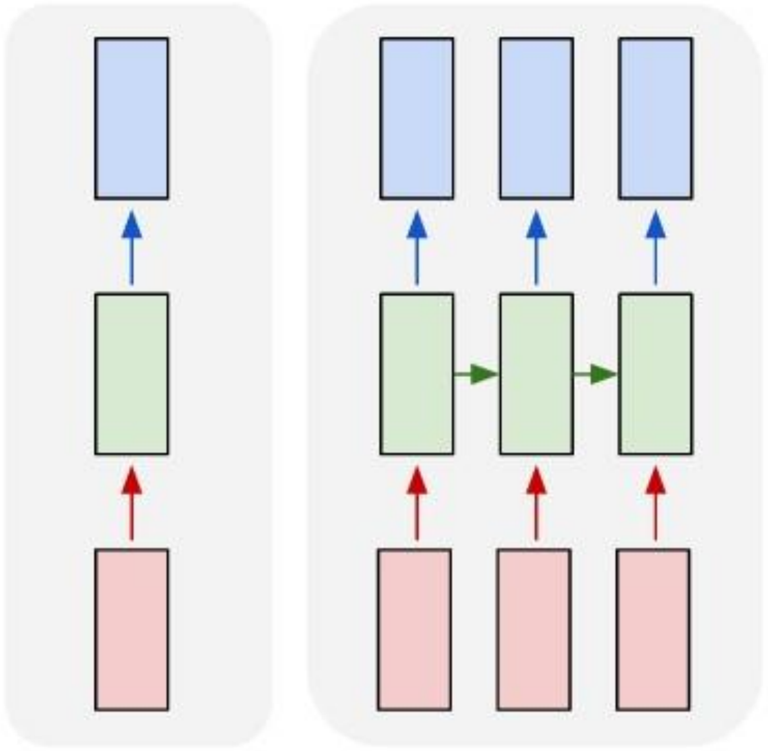


- Up to now
  - Simple neural network structure: 1-to-1 mapping of inputs to outputs
- Recurrent Neural Networks
  - Generalize this to arbitrary mappings

Image source: Andrej Karpathy

Recap: Recurrent Neural Networks (RNNs)

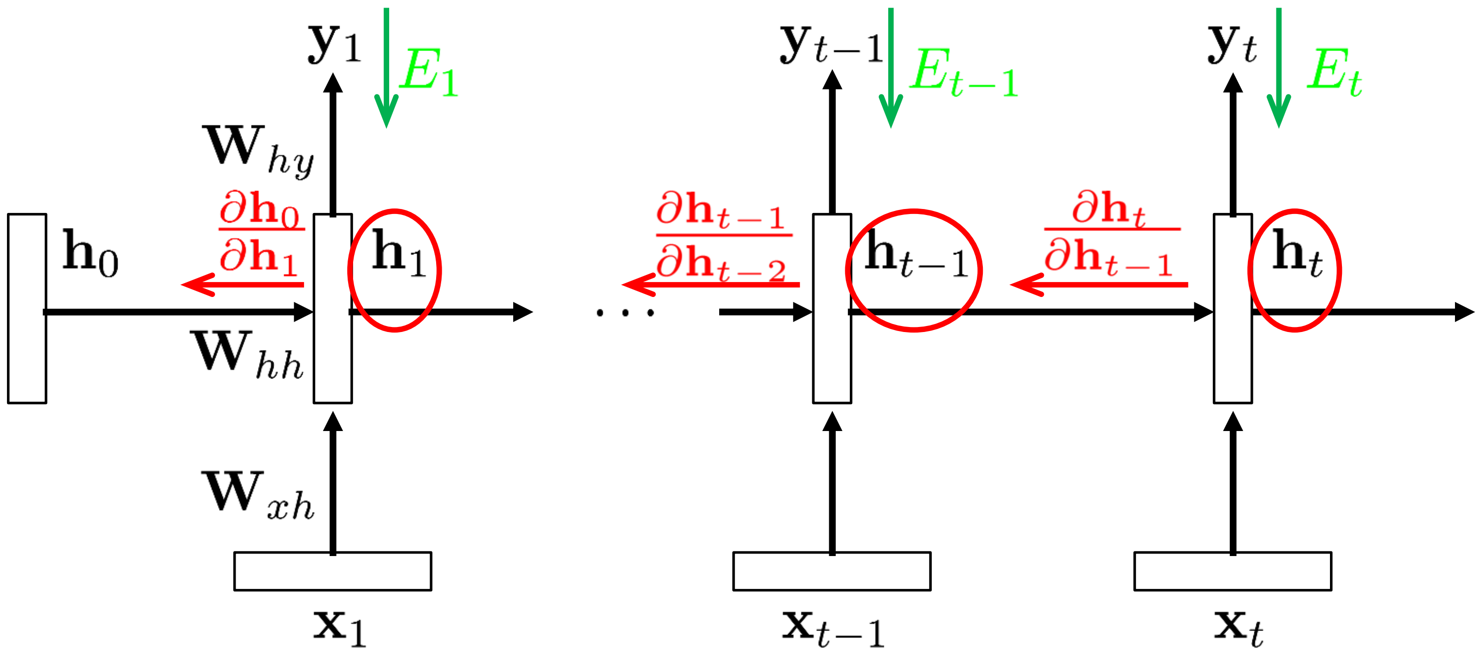
- RNNs are regular NNs whose hidden units have additional connections over time.
  - You can unroll them to create a network that extends over time.
  - When you do this, keep in mind that the weights for the hidden are shared between temporal layers.



- RNNs are very powerful
  - With enough neurons and time, they can compute anything that can be computed by your computer.

Image source: Andrej Karpathy

Recap: Backpropagation Through Time (BPTT)



- Configuration

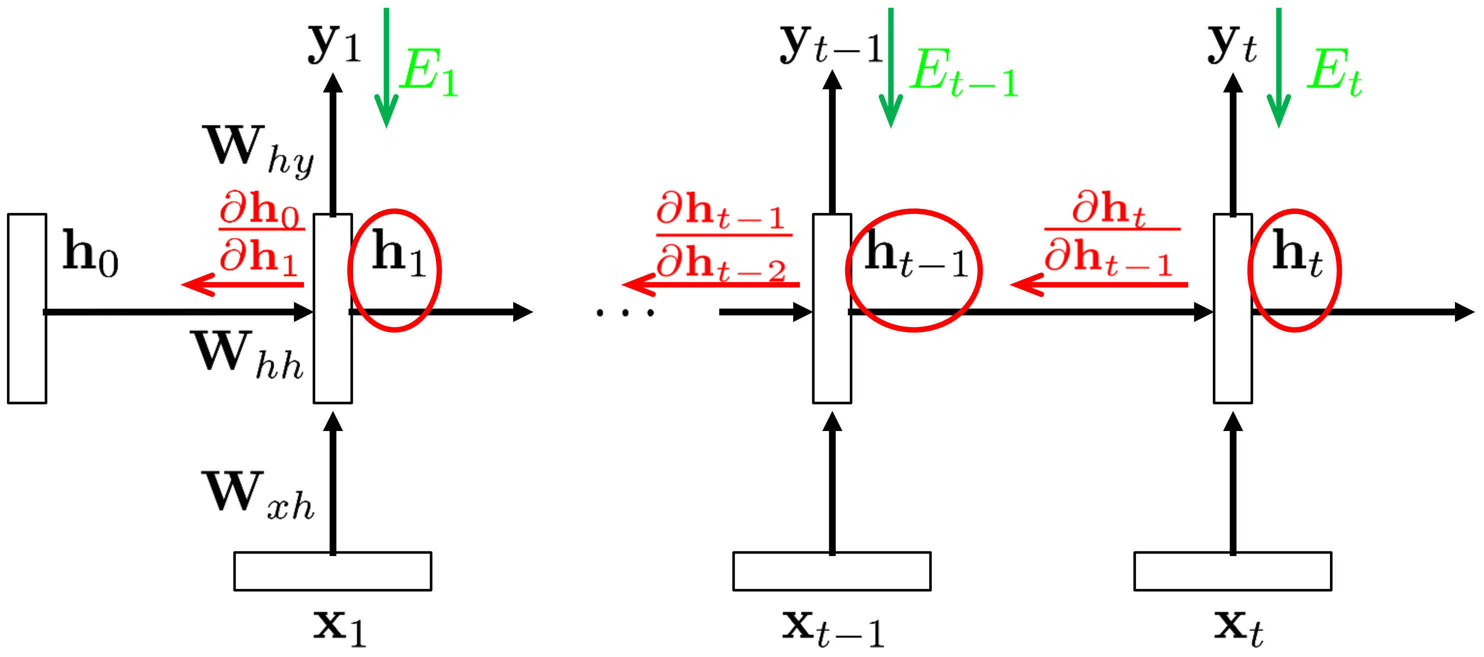
$$\mathbf{h}_t = \sigma\left(\mathbf{W}_{xh}\mathbf{x}_t + \mathbf{W}_{hh}\mathbf{h}_{t-1} + b\right)$$

$$\hat{\mathbf{y}}_t = \mathrm{softmax}\left(\mathbf{W}_{hy}\mathbf{h}_t\right)$$

- Backpropagated gradient
  - For weight w_{ij}:

$$\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \le k \le t} \left(\frac{\partial E_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial^+ h_k}{\partial w_{ij}} \right)$$

Recap: Backpropagation Through Time (BPTT)

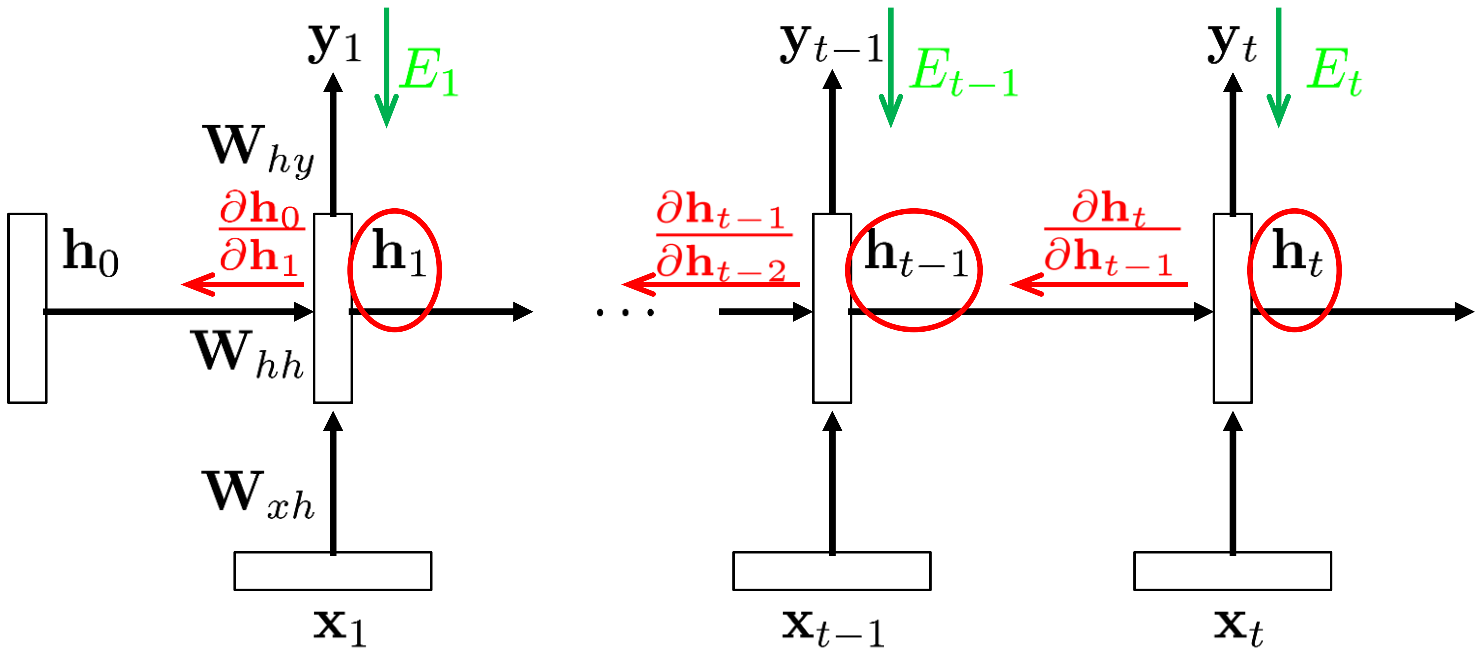


- Analyzing the terms
  - For weight w_{ij}:

$$\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \le k \le t} \left(\frac{\partial E_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial^+ h_k}{\partial w_{ij}} \right)$$

  - This is the “immediate” partial derivative (with $\mathbf{h}_{k\text{-}1}$ as constant)

Recap: Backpropagation Through Time (BPTT)



- Analyzing the terms
  - For weight w_{ij}:
    $$\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \le k \le t} \left(\frac{\partial E_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial^+ h_k}{\partial w_{ij}} \right)$$
  - Propagation term:
    $$\frac{\partial h_t}{\partial h_k} = \prod_{t \ge i > k} \frac{\partial \mathbf{h}_i}{\partial \mathbf{h}_{i-1}}$$

Recap: Backpropagation Through Time (BPTT)

see Exercise 6.1

- Summary
  - Backpropagation equations

$$E = \sum_{1 \leq t \leq T} E_t$$

$$\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \leq k \leq t} \left(\frac{\partial E_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial^+ h_k}{\partial w_{ij}} \right)$$

$$\frac{\partial h_t}{\partial h_k} = \prod_{t \geq i > k} \frac{\partial \mathbf{h}_i}{\partial \mathbf{h}_{i-1}} = \prod_{t \geq i > k} \mathbf{W}_{hh}^\top diag\left(\sigma'(\mathbf{h}_{i-1})\right)$$

  - Remaining issue: how to set the initial state $\mathbf{h}_0$?

$\Rightarrow$ Learn this together with all the other parameters.

Recap: Exploding / Vanishing Gradient Problem

- BPTT equations:

$$\frac{\partial E_t}{\partial w_{ij}} = \sum_{1 \le k \le t} \left(\frac{\partial E_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial^+ h_k}{\partial w_{ij}} \right)$$

$$\frac{\partial h_t}{\partial h_k} = \prod_{t \ge i > k} \frac{\partial \mathbf{h}_i}{\partial \mathbf{h}_{i-1}} = \prod_{t \ge i > k} \mathbf{W}_{hh}^{\top} diag\left(\sigma'(\mathbf{h}_{i-1})\right)$$

$$= \left(\mathbf{W}_{hh}^{\top}\right)^l$$

(if t goes to infinity and $l = t - k$.)

$\Rightarrow$ We are effectively taking the weight matrix to a high power.

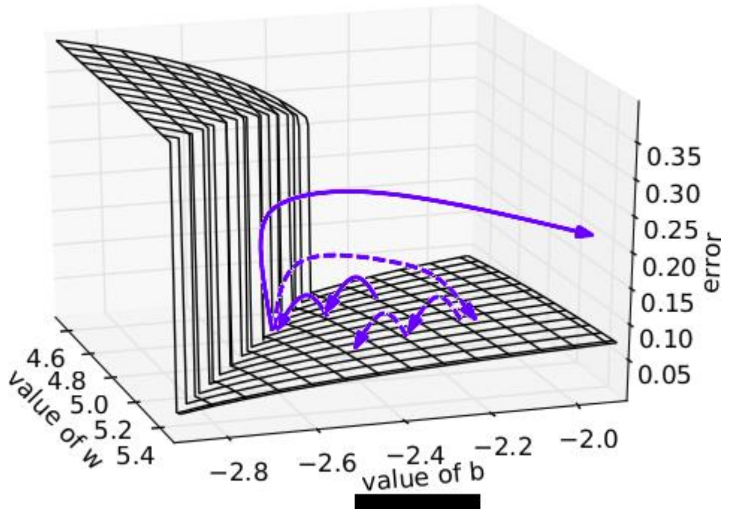
- The result will depend on the eigenvalues of $\mathbf{W}_{hh}$.
  - Largest eigenvalue > 1 $\Rightarrow$ Gradients *may* explode.
  - Largest eigenvalue < 1 $\Rightarrow$ Gradients *will* vanish.
  - This is very bad...

Recap: Gradient Clipping

- Trick to handle exploding gradients
  - If the gradient is larger than a threshold, clip it to that threshold.

Algorithm 1 Pseudo-code

```
$\hat{\mathbf{g}} \leftarrow \frac{\partial \mathcal{E}}{\partial \theta}$
if $\|\hat{\mathbf{g}}\| \geq threshold$ then
    $\hat{\mathbf{g}} \leftarrow \frac{threshold}{\|\hat{\mathbf{g}}\|} \hat{\mathbf{g}}$
end if
```

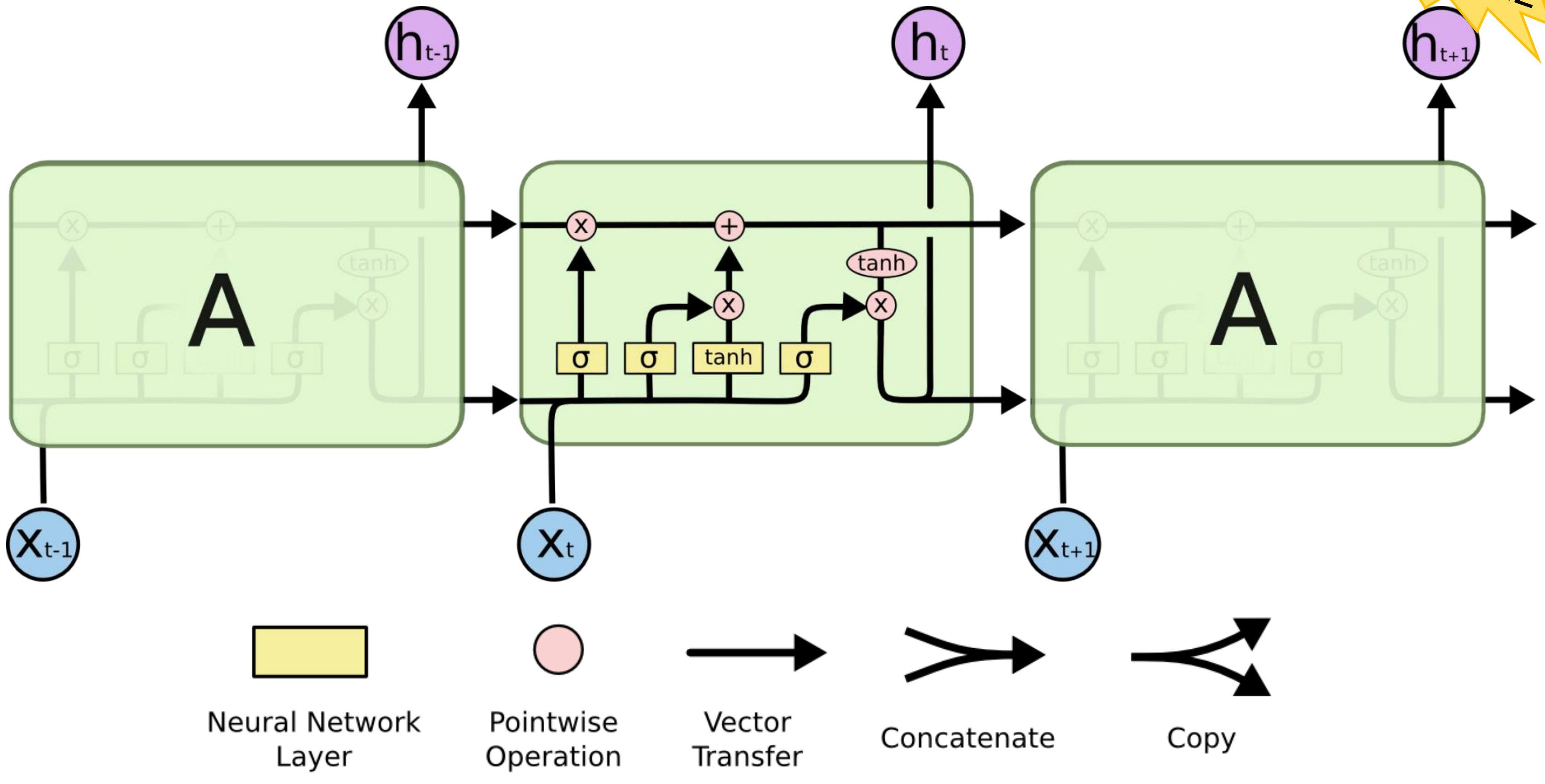


  - This makes a big difference in RNNs

Slide adapted from Richard Socher

Recap: Long Short-Term Memory

see Exercise 6.2



- LSTMs
  - Inspired by the design of memory cells
  - Each module has 4 layers, interacting in a special way.

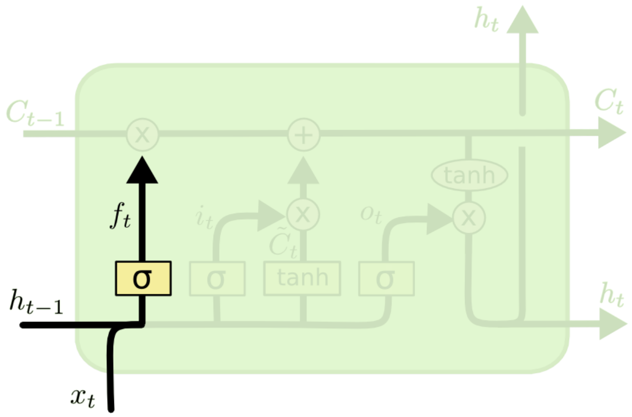
Image source: Christopher Olah, http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Recap: Elements of LSTMs

- Forget gate layer
  - Look at $\mathbf{h}_{t\text{-}1}$ and $\mathbf{x}_t$ and output a number between 0 and 1 for each dimension in the cell state $\mathbf{C}_{t\text{-}1}$.

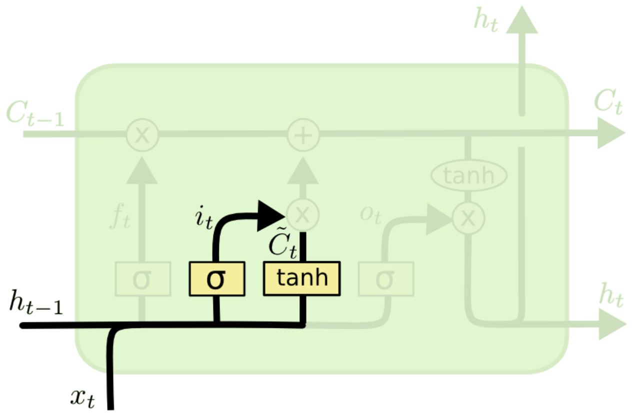
    0: completely delete this,

    1: completely keep this.



$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] \; + \; b_f\right)$$

- Update gate layer
  - Decide what information to store in the cell state.
  - Sigmoid network (input gate layer) decides which values are updated.
  - tanh layer creates a vector of new candidate values that could be added to the state.



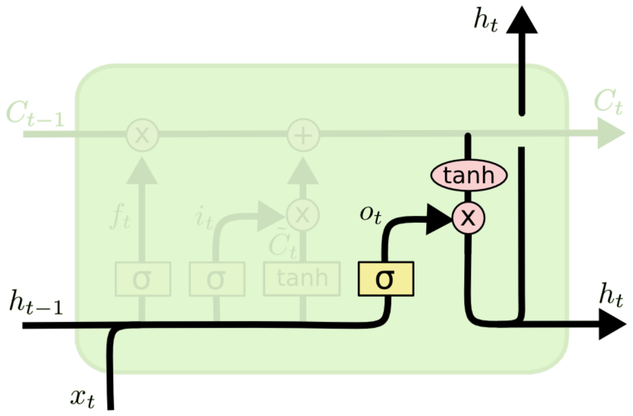
$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \; + \; b_i\right)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \; + \; b_C)$$

Source: Christopher Olah, http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Recap: Elements of LSTMs

- Output gate layer
  - Output is a filtered version of our gate state.
  - First, apply sigmoid layer to decide what parts of the cell state to output.
  - Then, pass the cell state through a tanh (to push the values to be between -1 and 1) and multiply it with the output of the sigmoid gate.



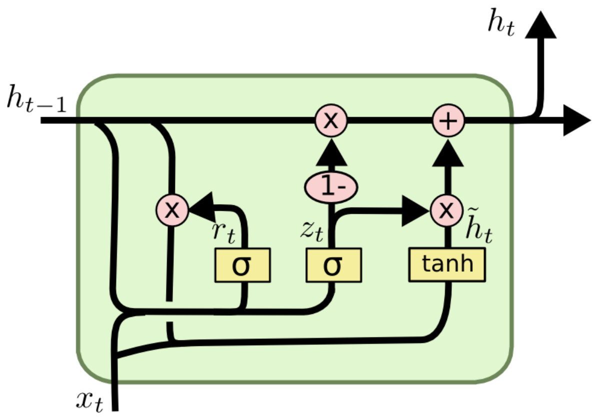
$$o_t = \sigma\left(W_o \left[h_{t-1}, x_t\right] + b_o\right)$$

$$h_t = o_t * \tanh\left(C_t\right)$$

Source: Christopher **Olah,** http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Recap: Gated Recurrent Units (GRU)

- Simpler model than LSTM
  - Combines the forget and input gates into a single update gate z_t.
  - Similar definition for a reset gate r_t, but with different weights.
  - In both cases, merge the cell state and hidden state.



$$z_t = \sigma\left(W_z \cdot [h_{t-1}, x_t]\right)$$

$$r_t = \sigma\left(W_r \cdot [h_{t-1}, x_t]\right)$$

$$\tilde{h}_t = \tanh\left(W \cdot [r_t * h_{t-1}, x_t]\right)$$

$$h_t = (1 - z_t) * h_{t-1} + z_t * \tilde{h}_t$$

- Empirical results
  - Both LSTM and GRU can learn much longer-term dependencies than regular RNNs
  - GRU performance similar to LSTM (no clear winner yet), but fewer parameters.

Source: Christopher Olah, http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Any More Questions?

Good luck for the exam!